

Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## pH-metric Result

logP (XH2 +) 1.38 ±1.07 (n=50)  
 logP (neutral XH) 3.14 ±0.01 (n=50)  
 logP (X -) -1.62

### 18C-01007 Points 1 to 30

M16\_octanol concentration factor 0.780  
 Carbonate 0.1052 mM  
 Acidity error 3.38405 mM

### 18C-01007 Points 31 to 58

M16\_octanol concentration factor 0.751  
 Carbonate 0.8332 mM  
 Acidity error 2.20126 mM

### 18C-01007 Points 59 to 86

M16\_octanol concentration factor 0.772  
 Carbonate 0.5481 mM  
 Acidity error 2.29676 mM

## Warnings and errors

Errors None  
 Warnings Excessive carbonate concentration present

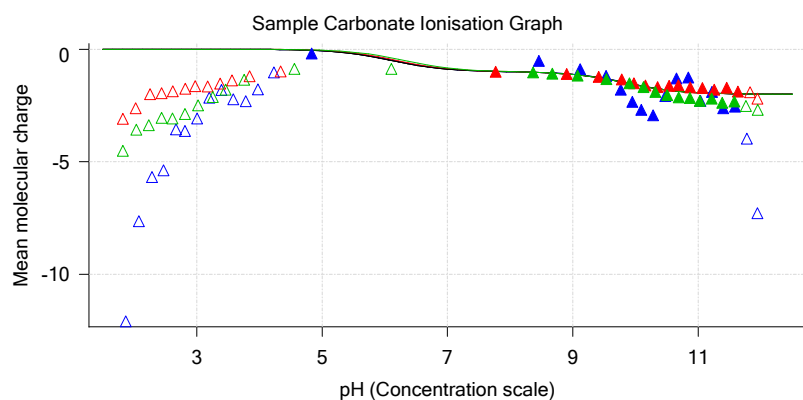
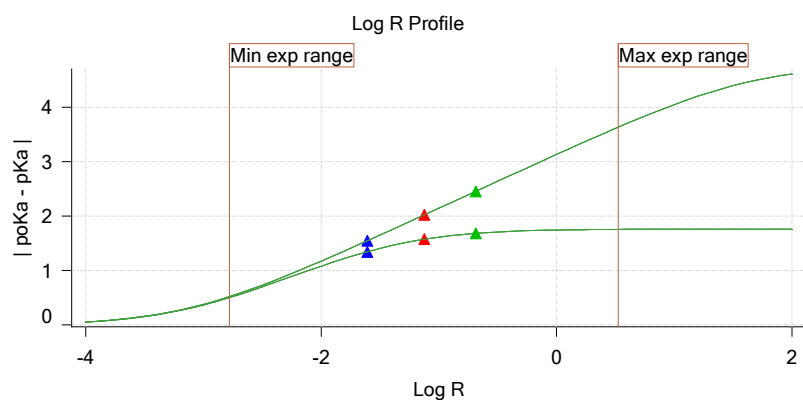
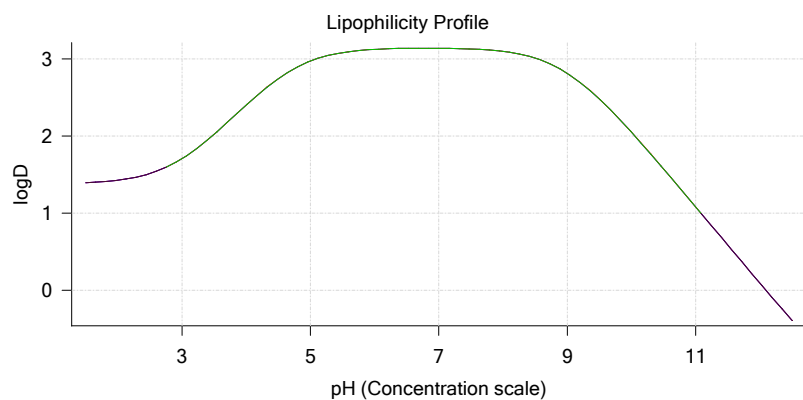
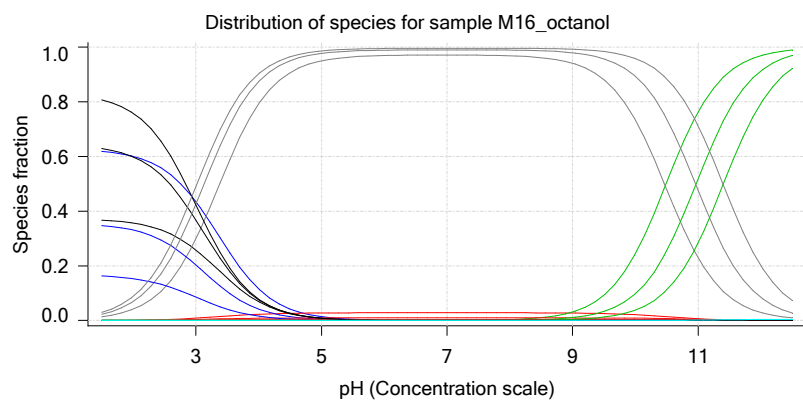
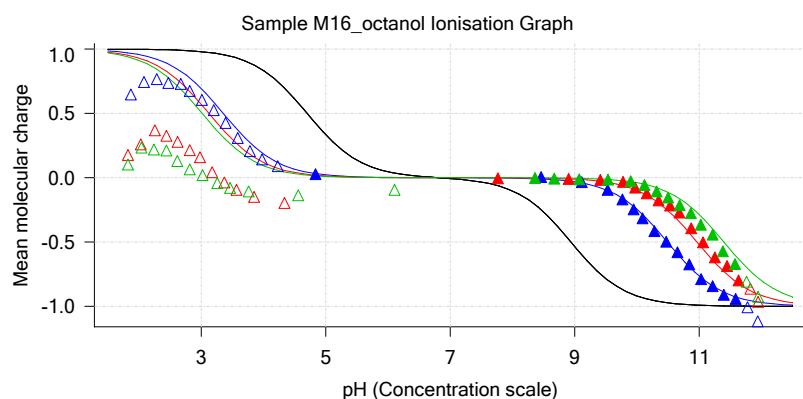
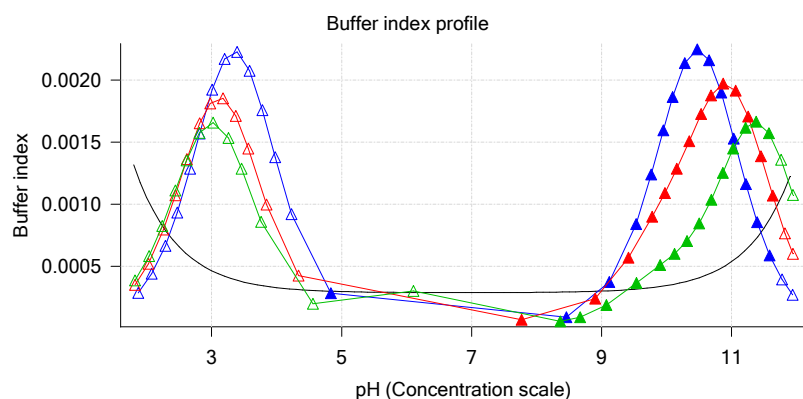
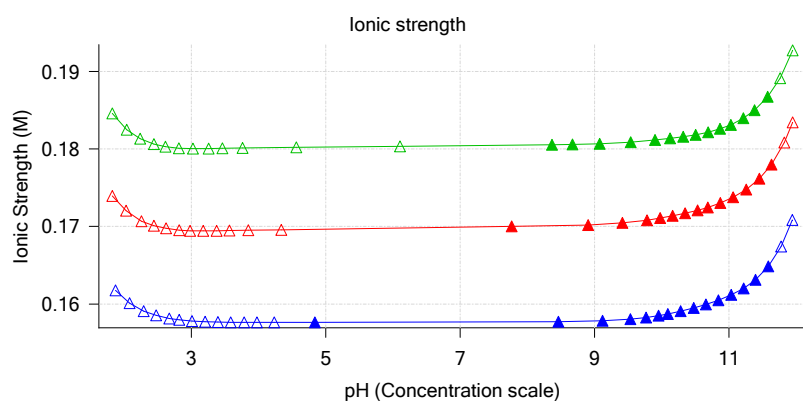
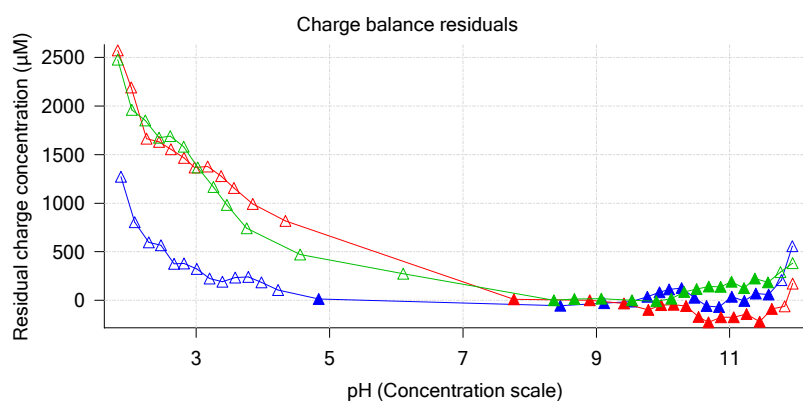
## Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	1.39	3.94 %	0.00 %	0.00 %	94.96 %	1.10 %	0.00 %	Stomach pH
1.200	1.39	3.92 %	0.00 %	0.00 %	94.35 %	1.73 %	0.00 %	
2.000	1.43	3.59 %	0.01 %	0.00 %	86.42 %	9.99 %	0.00 %	
3.000	1.71	1.89 %	0.04 %	0.00 %	45.50 %	52.58 %	0.00 %	Blood pH
4.000	2.40	0.33 %	0.07 %	0.00 %	7.93 %	91.67 %	0.00 %	
5.000	2.97	0.04 %	0.07 %	0.00 %	0.86 %	99.04 %	0.00 %	
6.000	3.12	0.00 %	0.07 %	0.00 %	0.09 %	99.84 %	0.00 %	
6.500	3.14	0.00 %	0.07 %	0.00 %	0.03 %	99.90 %	0.00 %	
7.000	3.14	0.00 %	0.07 %	0.00 %	0.01 %	99.92 %	0.00 %	
7.400	3.13	0.00 %	0.07 %	0.00 %	0.00 %	99.92 %	0.00 %	
8.000	3.10	0.00 %	0.07 %	0.01 %	0.00 %	99.92 %	0.00 %	
9.000	2.81	0.00 %	0.07 %	0.08 %	0.00 %	99.84 %	0.00 %	
10.000	2.05	0.00 %	0.07 %	0.82 %	0.00 %	99.09 %	0.02 %	
11.000	1.08	0.00 %	0.07 %	7.59 %	0.00 %	92.16 %	0.18 %	
12.000	0.09	0.00 %	0.04 %	44.66 %	0.00 %	54.23 %	1.07 %	

Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

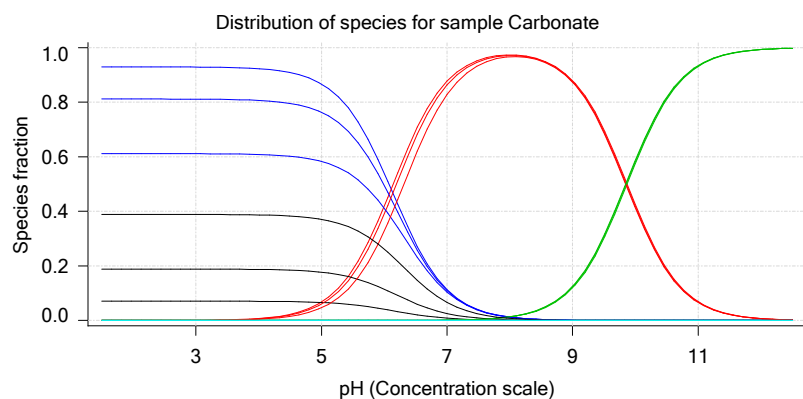
## Graphs



Sample name: **M16\_octanol**  
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 Instrument ID: **T312060**

## Graphs (continued)



Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## pH-metric high logP Titration 1 of 3 18C-01007 Points 1 to 30

### Overall results

RMSD 0.139  
 Average ionic strength 0.160 M  
 Average temperature 25.0°C  
 Partition ratio 0.0246 : 1  
 Analyte concentration range 4642.2 µM to 4978.9 µM  
 Total points considered 15 of 30

### Warnings and errors

Errors None  
 Warnings Excessive acidity error present

### Four-Plus parameters

Alpha 0.130 3/1/2018 9:25:33 AM C:\Sirius\_T3\HCl18B27.t3r  
 S 0.9970 3/1/2018 9:25:33 AM C:\Sirius\_T3\HCl18B27.t3r  
 jH 0.8 3/1/2018 9:25:33 AM C:\Sirius\_T3\HCl18B27.t3r  
 jOH -0.4 3/1/2018 9:25:33 AM C:\Sirius\_T3\HCl18B27.t3r

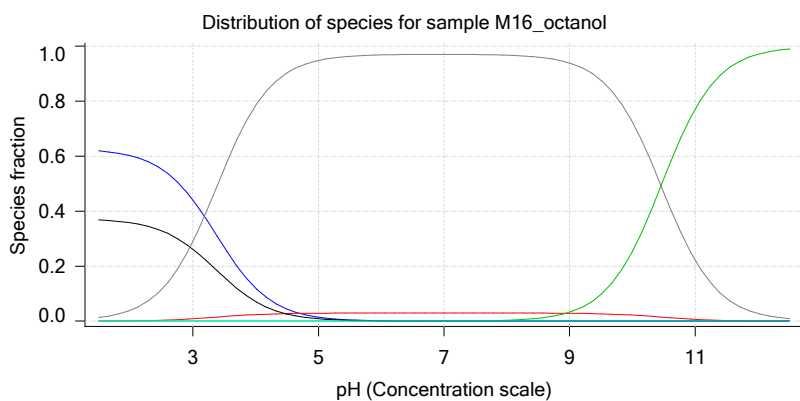
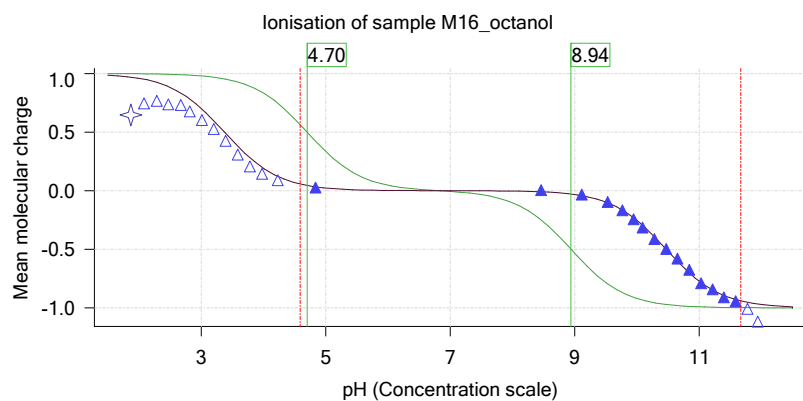
### Titrants

0.50 M HCl 0.993513 3/1/2018 9:25:34 AM C:\Sirius\_T3\HCl18B27.t3r  
 0.50 M KOH 0.999845 3/1/2018 9:25:34 AM C:\Sirius\_T3\KOH18B27.t3r

### Sample

M16\_octanol concentration factor 0.780  
 Base pKa 1 4.70  
 Acid pKa 2 8.94  
 logP (XH<sub>2</sub><sup>+</sup>) 1.38  
 logP (neutral XH) 3.12  
 logP (X<sup>-</sup>) -1.62

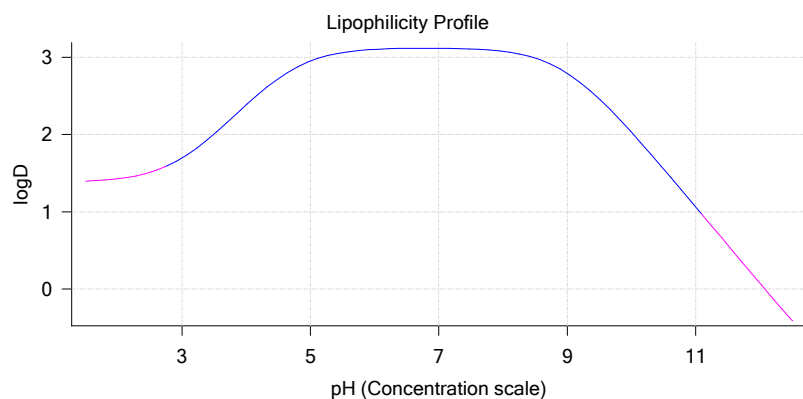
### Sample graphs



Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Sample graphs (continued)



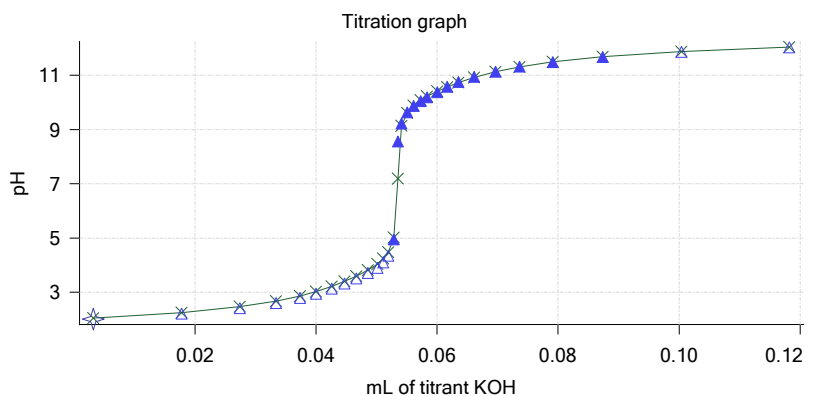
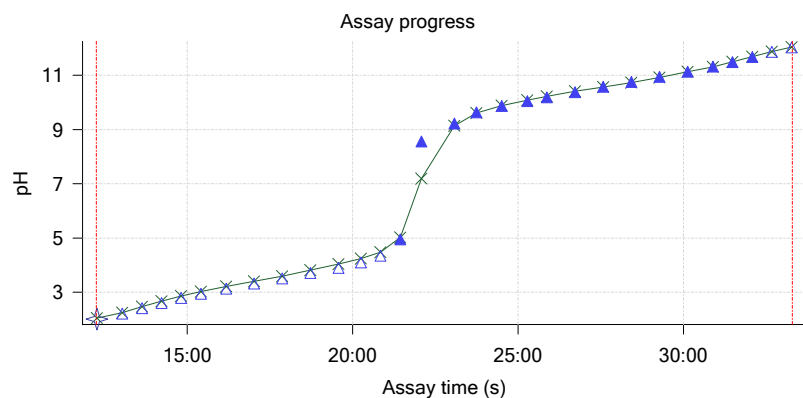
## Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	1.39	62.47 %	0.01 %	0.00 %	37.11 %	0.41 %	0.00 %	Stomach pH
1.200	1.39	62.31 %	0.02 %	0.00 %	37.02 %	0.65 %	0.00 %	
2.000	1.43	60.18 %	0.12 %	0.00 %	35.75 %	3.94 %	0.00 %	
3.000	1.70	44.07 %	0.88 %	0.00 %	26.18 %	28.87 %	0.00 %	
4.000	2.38	11.99 %	2.39 %	0.00 %	7.12 %	78.50 %	0.00 %	Blood pH
5.000	2.95	1.45 %	2.89 %	0.00 %	0.86 %	94.80 %	0.00 %	
6.000	3.10	0.15 %	2.95 %	0.00 %	0.09 %	96.81 %	0.00 %	
6.500	3.12	0.05 %	2.95 %	0.01 %	0.03 %	96.96 %	0.00 %	
7.000	3.12	0.01 %	2.95 %	0.03 %	0.01 %	96.99 %	0.00 %	
7.400	3.11	0.01 %	2.95 %	0.09 %	0.00 %	96.95 %	0.00 %	
8.000	3.08	0.00 %	2.95 %	0.34 %	0.00 %	96.71 %	0.00 %	
9.000	2.79	0.00 %	2.86 %	3.28 %	0.00 %	93.86 %	0.00 %	
10.000	2.03	0.00 %	2.21 %	25.34 %	0.00 %	72.44 %	0.01 %	
11.000	1.06	0.00 %	0.67 %	77.21 %	0.00 %	22.08 %	0.05 %	
12.000	0.07	0.00 %	0.08 %	97.08 %	0.00 %	2.78 %	0.06 %	

## Carbonate and acidity

Carbonate 0.105 mM  
 Acidity error 3.384 mM

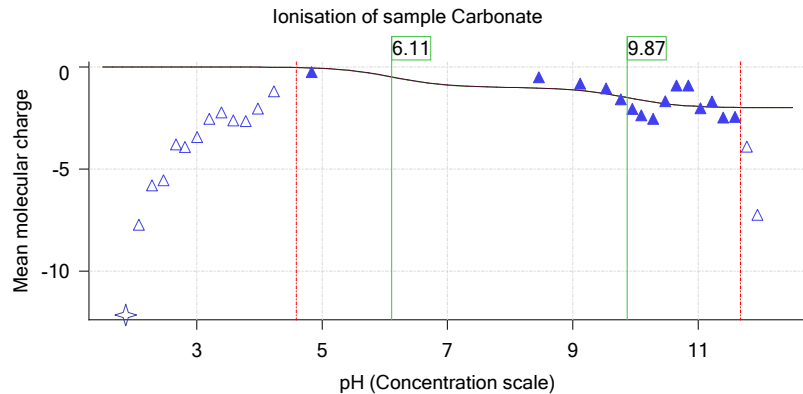
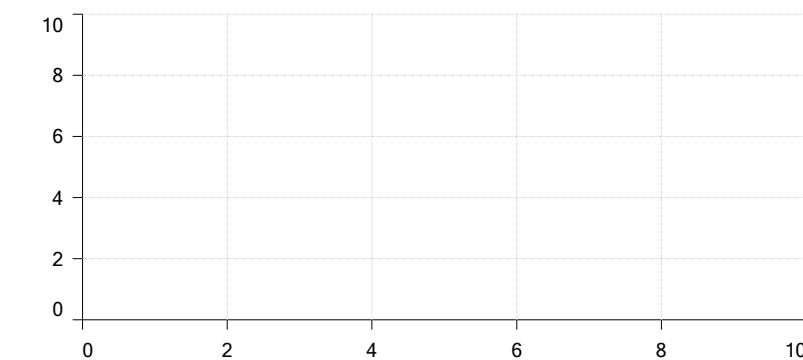
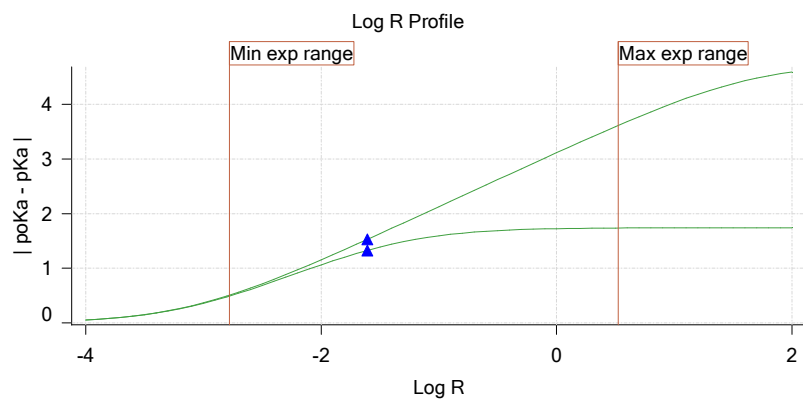
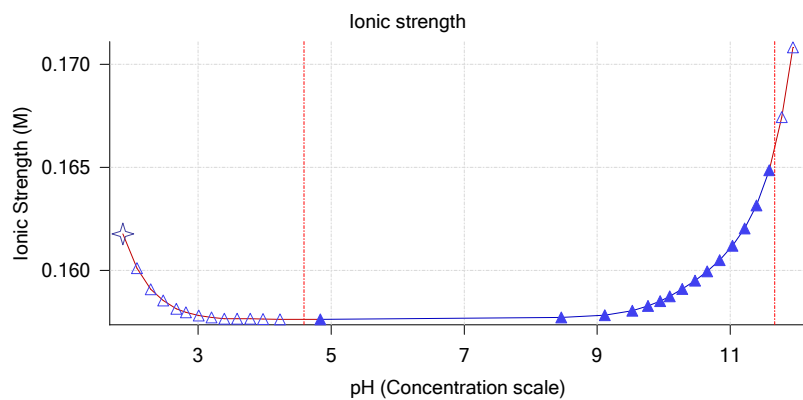
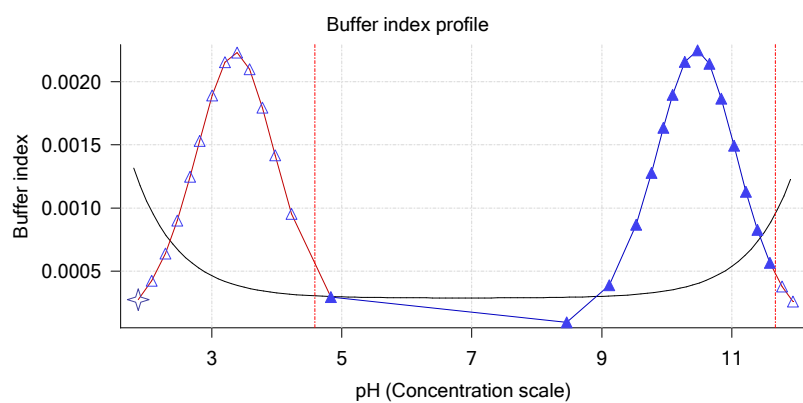
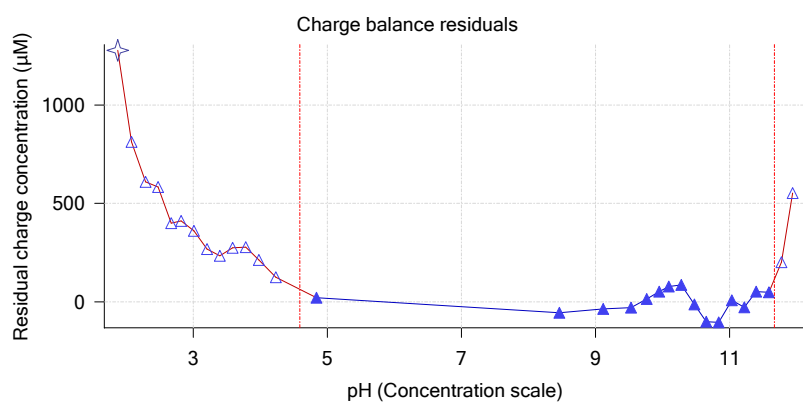
## Other graphs



Sample name: **M16\_octanol**  
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 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Other graphs (continued)



Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## pH-metric high logP Titration 2 of 3 18C-01007 Points 31 to 58





### Overall results

RMSD 0.048  
 Average ionic strength 0.173 M  
 Average temperature 25.0°C  
 Partition ratio 0.0752 : 1  
 Analyte concentration range 3835.8 µM to 4100.8 µM  
 Total points considered 14 of 28



### Warnings and errors

Errors None  
 Warnings One or more logP values out of range  
 Excessive carbonate concentration present  
 Excessive acidity error present







### Four-Plus parameters

	Alpha	0.130	3/1/2018 9:25:33 AM	C:\Sirius_T3\HCl18B27.t3r
	S	0.9970	3/1/2018 9:25:33 AM	C:\Sirius_T3\HCl18B27.t3r
	jH	0.8	3/1/2018 9:25:33 AM	C:\Sirius_T3\HCl18B27.t3r
	jOH	-0.4	3/1/2018 9:25:33 AM	C:\Sirius_T3\HCl18B27.t3r

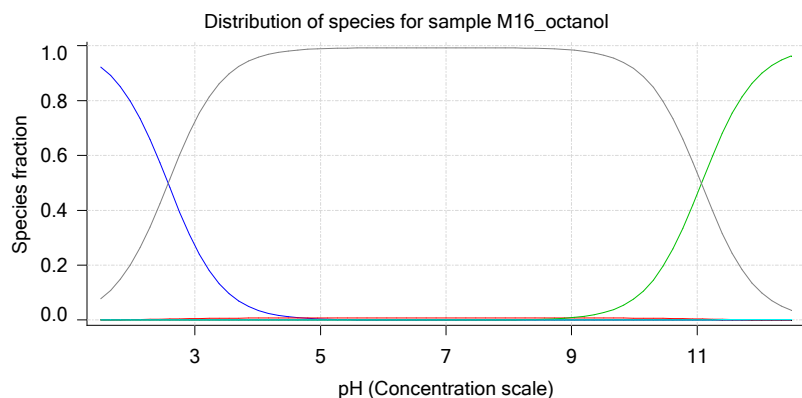
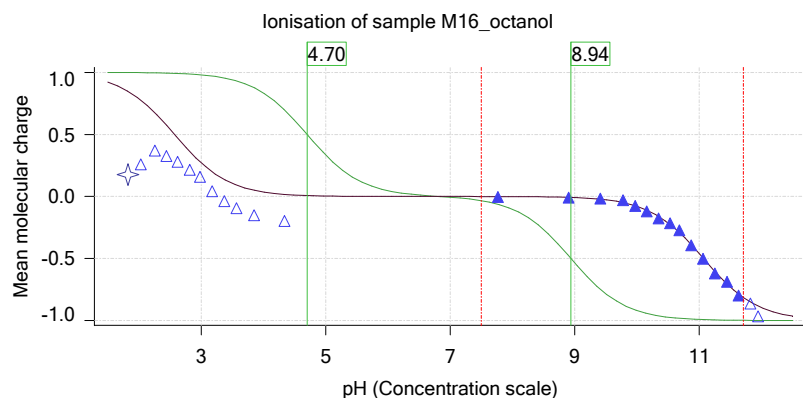
### Titants

	0.50 M HCl	0.993513	3/1/2018 9:25:34 AM	C:\Sirius_T3\HCl18B27.t3r
	0.50 M KOH	0.999845	3/1/2018 9:25:34 AM	C:\Sirius_T3\KOH18B27.t3r

### Sample

	M16_octanol concentration factor	0.751
	Base pKa 1	4.70
	Acid pKa 2	8.94
	logP (XH <sub>2</sub> <sup>+</sup> )	-5.98
	logP (neutral XH)	3.25
	logP (X <sup>-</sup> )	-1.62

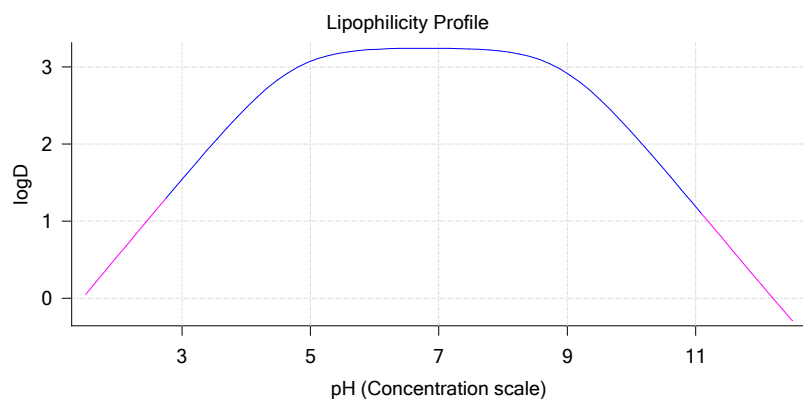
### Sample graphs



Sample name: **M16\_octanol**  
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 Assay ID: **18C-01007**  
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 Analyst: **Pion**  
 Instrument ID: **T312060**

## Sample graphs (continued)



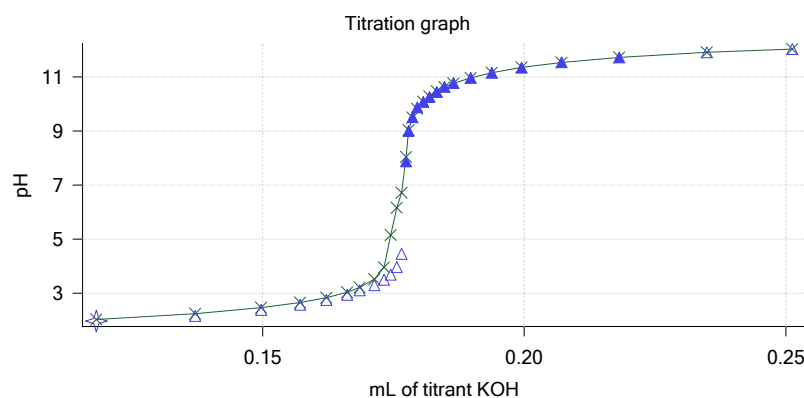
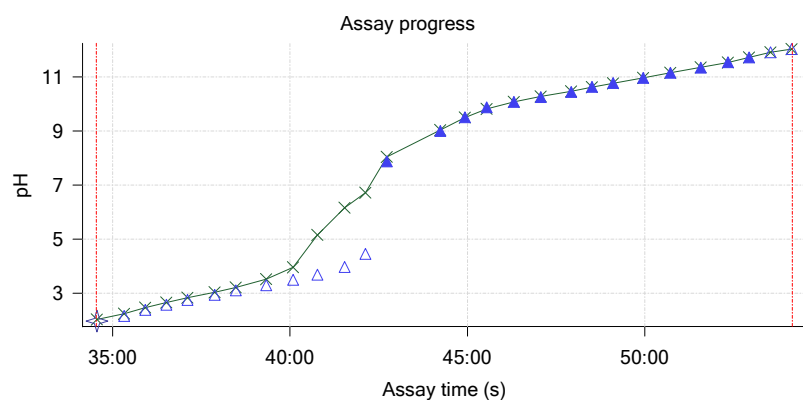
## Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	-0.45	97.38 %	0.02 %	0.00 %	0.00 %	2.60 %	0.00 %	Stomach pH
1.200	-0.25	95.91 %	0.03 %	0.00 %	0.00 %	4.06 %	0.00 %	
2.000	0.55	78.80 %	0.16 %	0.00 %	0.00 %	21.04 %	0.00 %	
3.000	1.54	27.10 %	0.54 %	0.00 %	0.00 %	72.36 %	0.00 %	
4.000	2.47	3.58 %	0.72 %	0.00 %	0.00 %	95.70 %	0.00 %	Blood pH
5.000	3.07	0.37 %	0.74 %	0.00 %	0.00 %	98.89 %	0.00 %	
6.000	3.23	0.04 %	0.74 %	0.00 %	0.00 %	99.22 %	0.00 %	
6.500	3.24	0.01 %	0.74 %	0.00 %	0.00 %	99.24 %	0.00 %	
7.000	3.24	0.00 %	0.74 %	0.01 %	0.00 %	99.25 %	0.00 %	
7.400	3.24	0.00 %	0.74 %	0.02 %	0.00 %	99.24 %	0.00 %	
8.000	3.20	0.00 %	0.74 %	0.09 %	0.00 %	99.17 %	0.00 %	
9.000	2.92	0.00 %	0.74 %	0.84 %	0.00 %	98.42 %	0.00 %	
10.000	2.15	0.00 %	0.68 %	7.85 %	0.00 %	91.45 %	0.01 %	
11.000	1.19	0.00 %	0.40 %	45.96 %	0.00 %	53.56 %	0.08 %	
12.000	0.20	0.00 %	0.08 %	89.35 %	0.00 %	10.41 %	0.16 %	

## Carbonate and acidity

Carbonate 0.833 mM  
 Acidity error 2.201 mM

## Other graphs

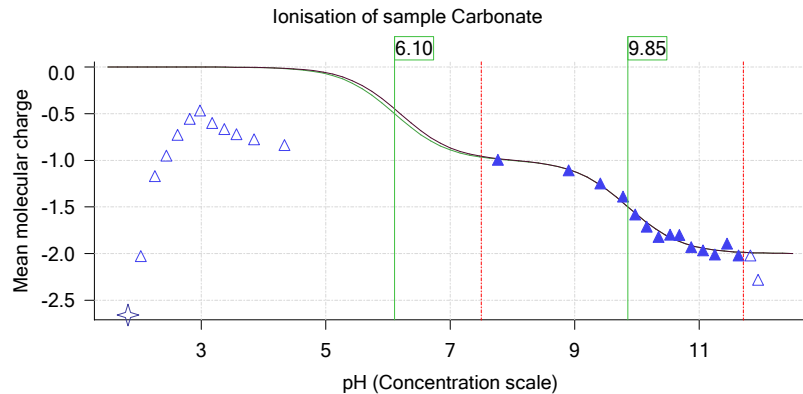
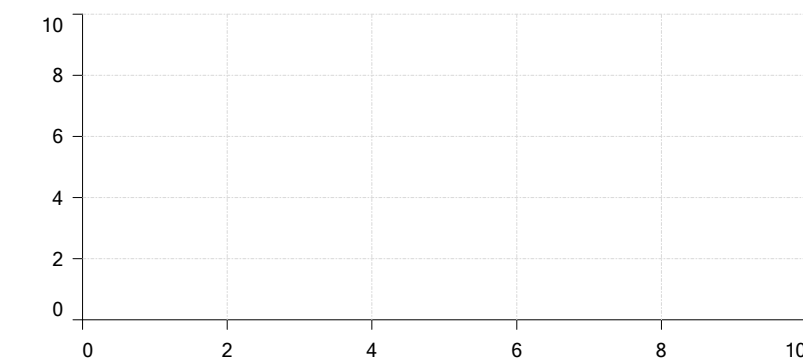
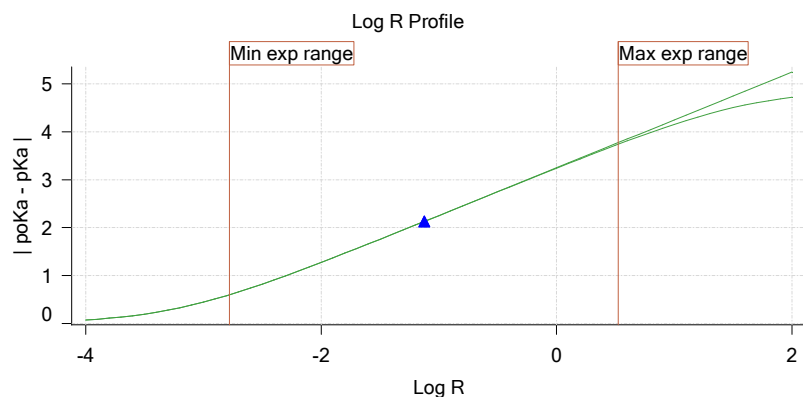
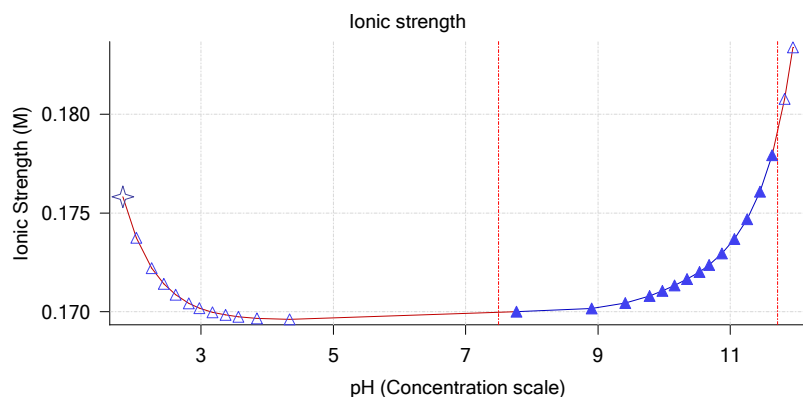
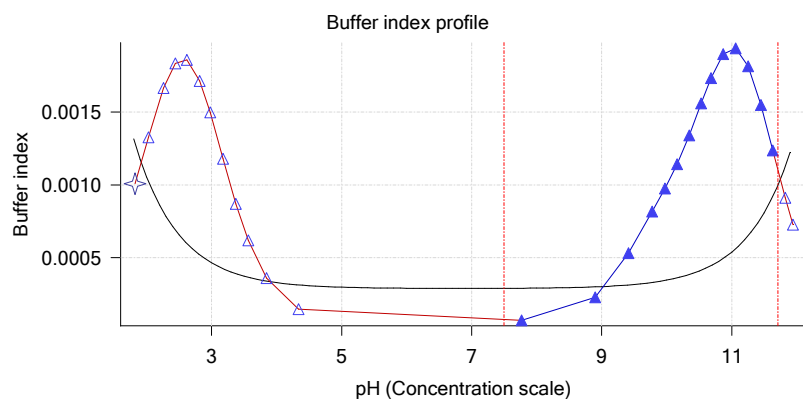
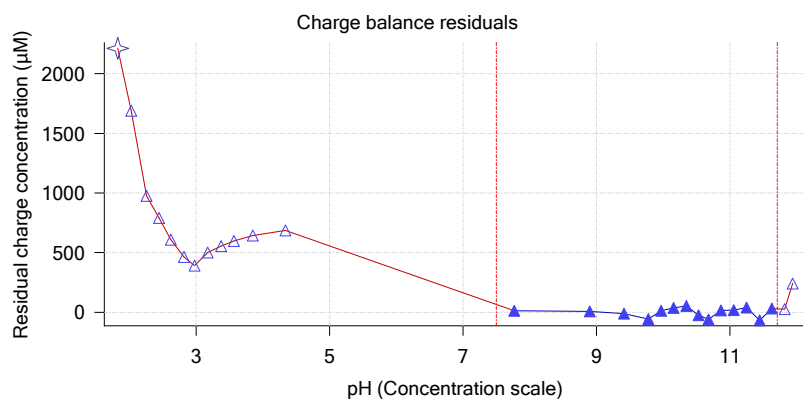




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 Analyst: **Pion**  
 Instrument ID: **T312060**

## Other graphs (continued)



Sample name: **M16\_octanol**  
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 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-01007 Points 59 to 86

## Overall results

RMSD 0.033  
 Average ionic strength 0.182 M  
 Average temperature 25.0°C  
 Partition ratio 0.2059 : 1  
 Analyte concentration range 2984.0 µM to 3160.6 µM  
 Total points considered 14 of 28

## Warnings and errors

Errors None  
 Warnings Excessive carbonate concentration present  
 Excessive acidity error present

## Four-Plus parameters

Alpha 0.130 3/1/2018 9:25:33 AM C:\Sirius\_T3\HCl18B27.t3r  
 S 0.9970 3/1/2018 9:25:33 AM C:\Sirius\_T3\HCl18B27.t3r  
 jH 0.8 3/1/2018 9:25:33 AM C:\Sirius\_T3\HCl18B27.t3r  
 jOH -0.4 3/1/2018 9:25:33 AM C:\Sirius\_T3\HCl18B27.t3r

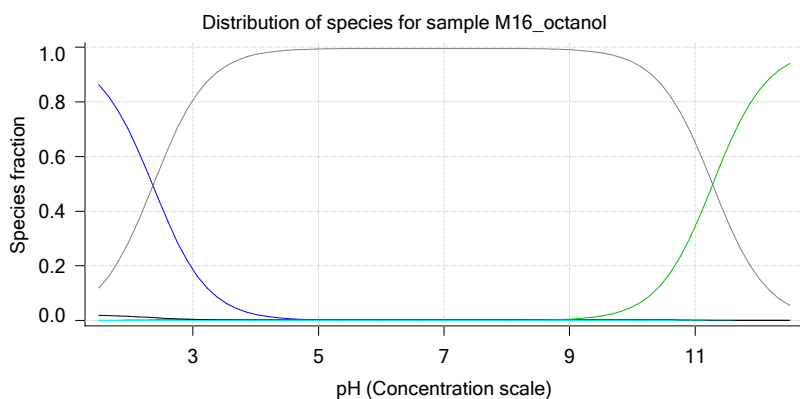
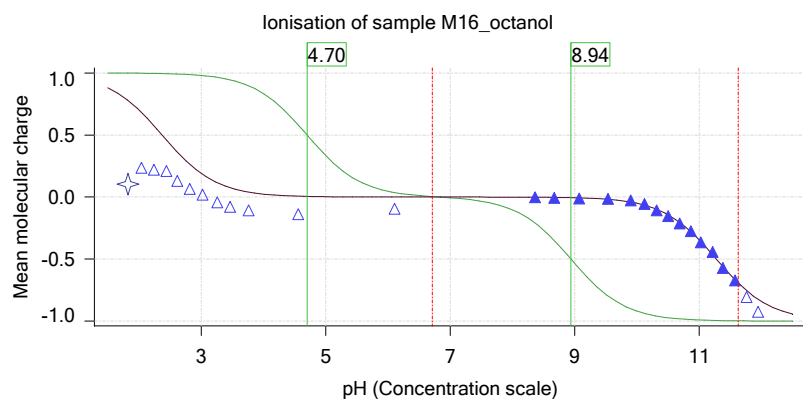
## Titants

0.50 M HCl 0.993513 3/1/2018 9:25:34 AM C:\Sirius\_T3\HCl18B27.t3r  
 0.50 M KOH 0.999845 3/1/2018 9:25:34 AM C:\Sirius\_T3\KOH18B27.t3r

## Sample

M16\_octanol concentration factor 0.772  
 Base pKa 1 4.70  
 Acid pKa 2 8.94  
 logP (XH<sub>2</sub><sup>+</sup>) -0.97  
 logP (neutral XH) 3.02  
 logP (X<sup>-</sup>) -1.62

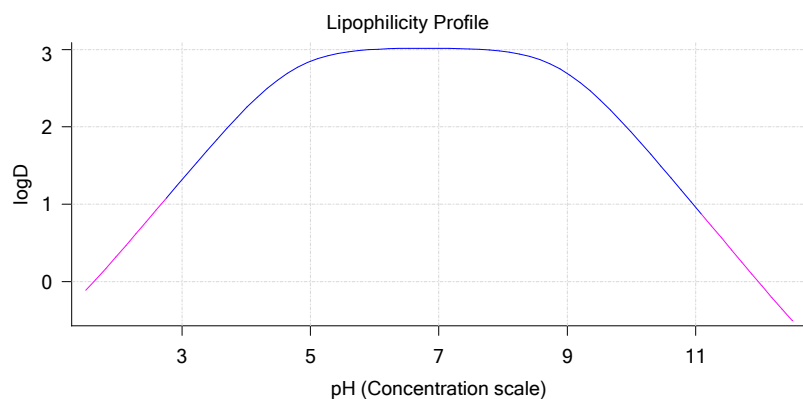
## Sample graphs



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Analyst: **Pion**  
Instrument ID: **T312060**

## Sample graphs (continued)



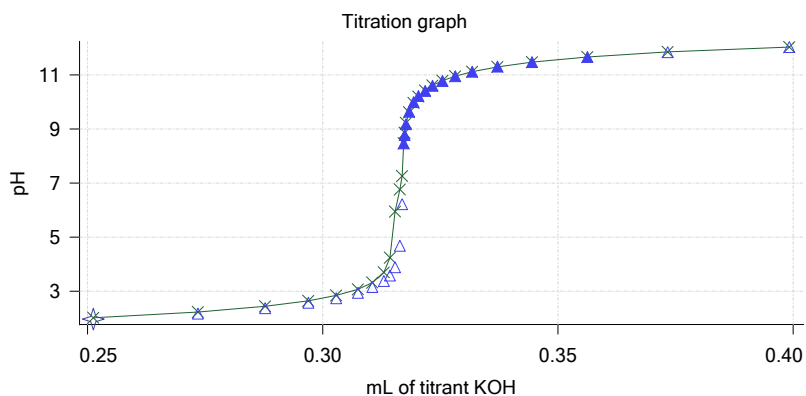
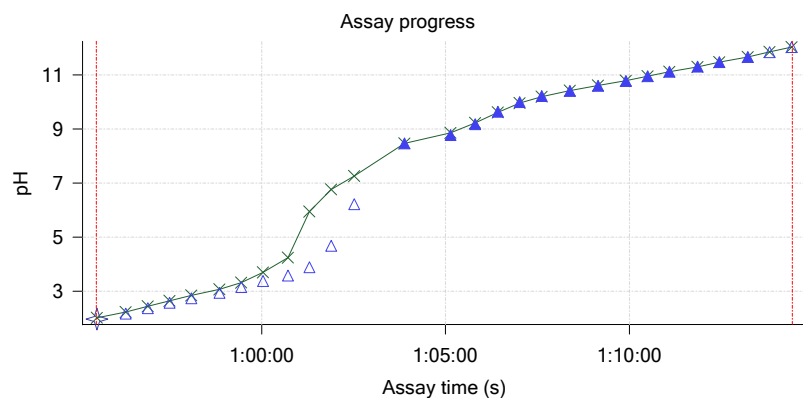
## Sample logD and percent species

pH	M16_octanol logD	M16_octanol M16_octanolH2	M16_octanol M16_octanolH	M16_octanol M16_octanol	M16_octanol M16_octanolH2*	M16_octanol M16_octanolH*	M16_octanol M16_octanol*	Comment
1.000	-0.50	93.84 %	0.02 %	0.00 %	2.07 %	4.07 %	0.00 %	Stomach pH
1.200	-0.36	91.65 %	0.03 %	0.00 %	2.02 %	6.29 %	0.00 %	
2.000	0.34	68.62 %	0.14 %	0.00 %	1.51 %	29.73 %	0.00 %	
3.000	1.32	18.60 %	0.37 %	0.00 %	0.41 %	80.61 %	0.00 %	
4.000	2.24	2.24 %	0.45 %	0.00 %	0.05 %	97.26 %	0.00 %	Blood pH
5.000	2.85	0.23 %	0.46 %	0.00 %	0.01 %	99.31 %	0.00 %	
6.000	3.00	0.02 %	0.46 %	0.00 %	0.00 %	99.52 %	0.00 %	
6.500	3.01	0.01 %	0.46 %	0.00 %	0.00 %	99.53 %	0.00 %	
7.000	3.02	0.00 %	0.46 %	0.01 %	0.00 %	99.53 %	0.00 %	
7.400	3.01	0.00 %	0.46 %	0.01 %	0.00 %	99.53 %	0.00 %	
8.000	2.98	0.00 %	0.46 %	0.05 %	0.00 %	99.49 %	0.00 %	
9.000	2.69	0.00 %	0.46 %	0.52 %	0.00 %	99.02 %	0.00 %	
10.000	1.93	0.00 %	0.44 %	5.00 %	0.00 %	94.54 %	0.02 %	
11.000	0.96	0.00 %	0.30 %	34.42 %	0.00 %	65.11 %	0.17 %	
12.000	-0.03	0.00 %	0.07 %	83.68 %	0.00 %	15.83 %	0.41 %	

## Carbonate and acidity

Carbonate 0.548 mM  
Acidity error 2.297 mM

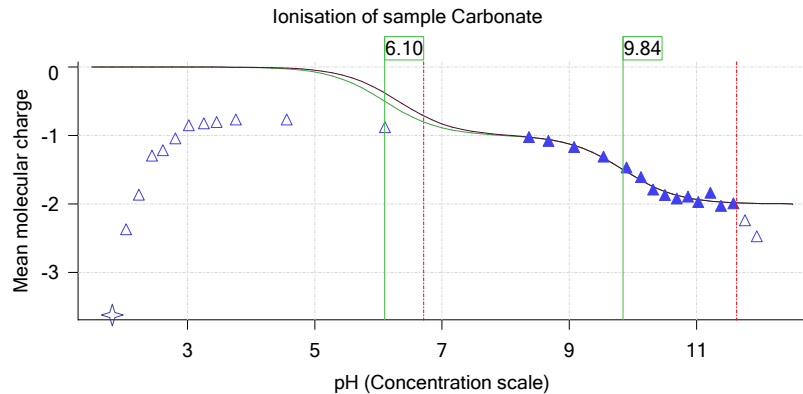
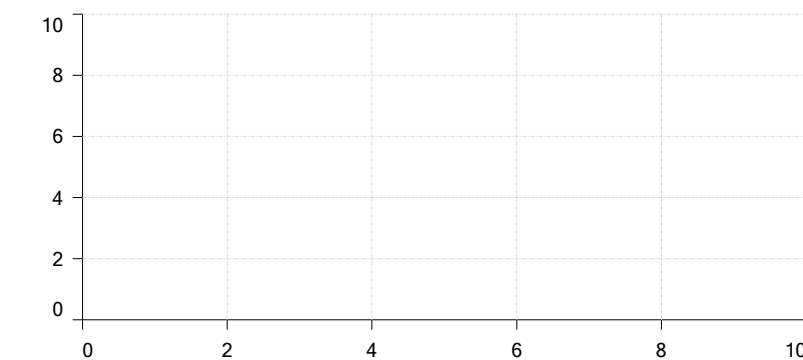
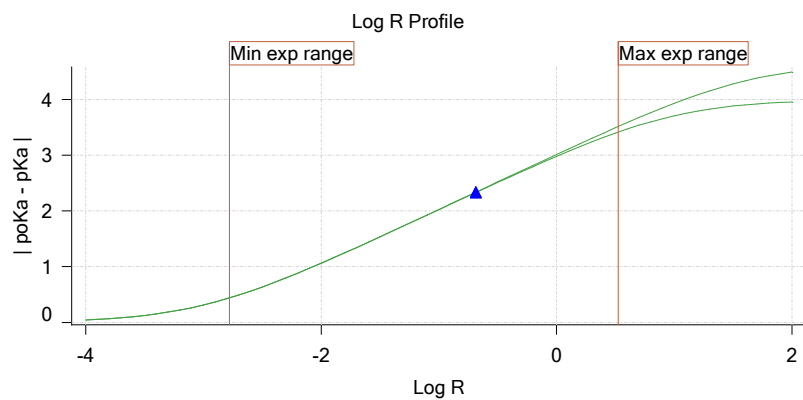
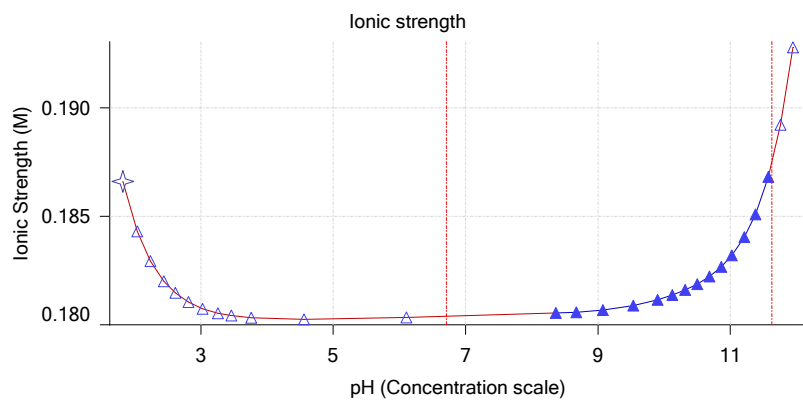
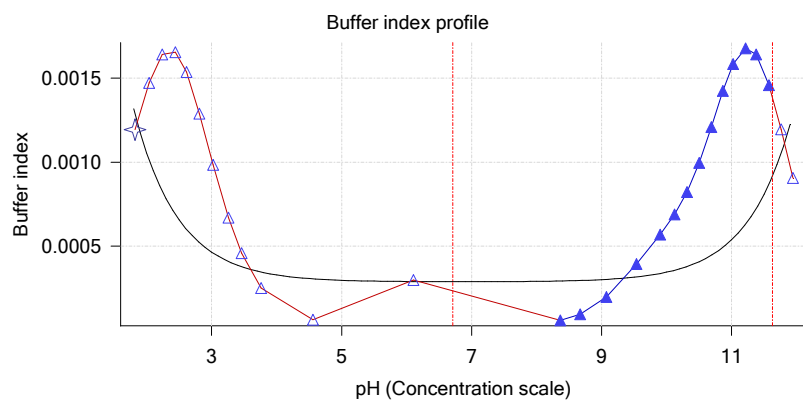
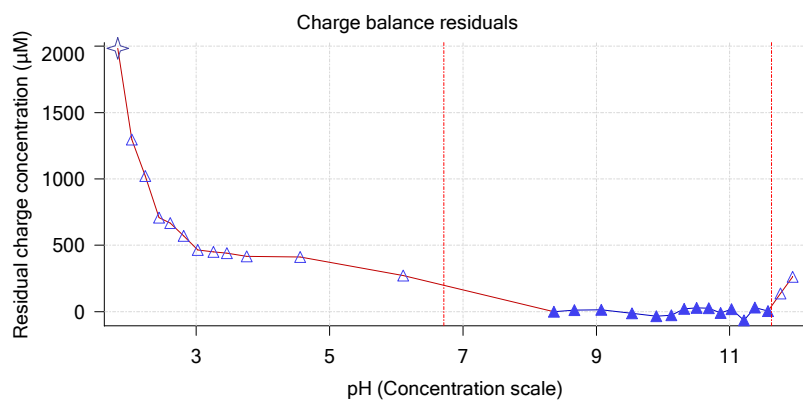
## Other graphs



Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Other graphs (continued)



Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M16_octanol	2/27/2018 6:14:13 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001660 g	2/28/2018 4:25:40 PM	User entered value
Formula weight	210.23 g/mol	2/27/2018 5:08:55 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	210.23	2/27/2018 5:08:55 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 5:08:55 PM	User entered value
Sample is a	Ampholyte	2/27/2018 5:08:55 PM	User entered value
pKa 1	4.70	2/27/2018 5:08:55 PM	User entered value
Type	Base	2/27/2018 5:08:55 PM	User entered value
pKa 2	8.94	2/27/2018 5:08:55 PM	User entered value
Type	Acid	2/27/2018 5:08:55 PM	User entered value
logp (XH2 +)	-0.97	2/27/2018 5:09:30 PM	User entered value
logP (neutral XH)	1.47	2/27/2018 5:09:44 PM	User entered value
logP (X -)	-1.62	2/27/2018 5:09:50 PM	User entered value

## Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
9:11.9	Initial pH = 3.56									
12:16.4	Data point 1	1.50000 mL	0.04271 mL	0.00320 mL	0.04000 mL	2.005	-0.00710	0.21574	0.00076	10.0 s
13:02.6	Data point 2	1.50000 mL	0.04271 mL	0.01778 mL	0.04000 mL	2.209	-0.00559	0.12657	0.00078	10.0 s
13:38.3	Data point 3	1.50000 mL	0.04271 mL	0.02740 mL	0.04000 mL	2.414	0.00086	0.04511	0.00020	10.0 s
14:13.8	Data point 4	1.50000 mL	0.04271 mL	0.03340 mL	0.04000 mL	2.598	-0.00678	0.14397	0.00088	10.0 s
14:49.3	Data point 5	1.50000 mL	0.04271 mL	0.03737 mL	0.04000 mL	2.793	-0.00172	0.13364	0.00023	10.0 s
15:24.9	Data point 6	1.50000 mL	0.04271 mL	0.03998 mL	0.04000 mL	2.938	-0.00257	0.34140	0.00022	10.0 s
16:10.7	Data point 7	1.50000 mL	0.04271 mL	0.04262 mL	0.04000 mL	3.130	-0.00330	0.56608	0.00022	10.0 s
17:01.6	Data point 8	1.50000 mL	0.04271 mL	0.04471 mL	0.04000 mL	3.323	-0.00522	0.10478	0.00080	10.0 s
17:52.6	Data point 9	1.50000 mL	0.04271 mL	0.04666 mL	0.04000 mL	3.513	-0.00408	0.55895	0.00027	10.0 s
18:43.6	Data point 10	1.50000 mL	0.04271 mL	0.04859 mL	0.04000 mL	3.704	-0.00652	0.61139	0.00041	10.0 s
19:34.5	Data point 11	1.50000 mL	0.04271 mL	0.05014 mL	0.04000 mL	3.901	-0.01015	0.66408	0.00061	10.0 s
20:15.1	Data point 12	1.50000 mL	0.04271 mL	0.05113 mL	0.04000 mL	4.094	-0.01157	0.56816	0.00076	10.0 s
20:50.6	Data point 13	1.50000 mL	0.04271 mL	0.05195 mL	0.04000 mL	4.347	-0.01522	0.64804	0.00093	10.5 s
21:26.5	Data point 14	1.50000 mL	0.04271 mL	0.05287 mL	0.04000 mL	4.951	-0.01799	0.87526	0.00095	13.0 s
22:05.0	Data point 15	1.50000 mL	0.04271 mL	0.05355 mL	0.04000 mL	8.563	-0.01946	0.98111	0.00097	34.0 s
23:04.4	Data point 16	1.50000 mL	0.04271 mL	0.05412 mL	0.04000 mL	9.218	-0.01863	0.95964	0.00094	14.5 s
23:44.4	Data point 17	1.50000 mL	0.04271 mL	0.05506 mL	0.04000 mL	9.631	-0.01929	0.94749	0.00098	10.5 s
24:30.7	Data point 18	1.50000 mL	0.04271 mL	0.05614 mL	0.04000 mL	9.865	-0.00801	0.59789	0.00051	10.5 s
25:17.1	Data point 19	1.50000 mL	0.04271 mL	0.05729 mL	0.04000 mL	10.048	-0.00508	0.13625	0.00068	10.0 s
25:52.5	Data point 20	1.50000 mL	0.04271 mL	0.05837 mL	0.04000 mL	10.190	-0.01000	0.36786	0.00081	10.0 s
26:43.4	Data point 21	1.50000 mL	0.04271 mL	0.06002 mL	0.04000 mL	10.377	-0.00716	0.23433	0.00073	10.0 s
27:34.3	Data point 22	1.50000 mL	0.04271 mL	0.06167 mL	0.04000 mL	10.570	-0.00128	0.01797	0.00047	10.0 s
28:25.3	Data point 23	1.50000 mL	0.04271 mL	0.06355 mL	0.04000 mL	10.750	-0.00897	0.69945	0.00053	10.0 s
29:16.4	Data point 24	1.50000 mL	0.04271 mL	0.06611 mL	0.04000 mL	10.936	-0.00376	0.05852	0.00077	10.0 s
30:07.5	Data point 25	1.50000 mL	0.04271 mL	0.06966 mL	0.04000 mL	11.128	-0.00187	0.33816	0.00016	10.0 s
30:53.5	Data point 26	1.50000 mL	0.04271 mL	0.07361 mL	0.04000 mL	11.313	-0.00175	0.34200	0.00015	10.0 s
31:29.0	Data point 27	1.50000 mL	0.04271 mL	0.07912 mL	0.04000 mL	11.488	0.00172	0.30827	0.00015	10.0 s
32:04.7	Data point 28	1.50000 mL	0.04271 mL	0.08739 mL	0.04000 mL	11.678	0.00337	0.74144	0.00019	10.0 s
32:40.4	Data point 29	1.50000 mL	0.04271 mL	0.10040 mL	0.04000 mL	11.865	-0.00296	0.02218	0.00098	10.0 s
33:16.3	Data point 30	1.50000 mL	0.04271 mL	0.11820 mL	0.04000 mL	12.028	0.01264	0.63373	0.00078	10.0 s
34:33.6	Data point 31	1.50000 mL	0.16729 mL	0.11820 mL	0.14000 mL	1.958	-0.01998	0.98240	0.00100	10.0 s
35:19.9	Data point 32	1.50000 mL	0.16729 mL	0.13709 mL	0.14000 mL	2.157	0.00252	0.43182	0.00019	10.0 s
35:55.6	Data point 33	1.50000 mL	0.16729 mL	0.14972 mL	0.14000 mL	2.384	0.00020	0.00012	0.00092	10.0 s
36:31.2	Data point 34	1.50000 mL	0.16729 mL	0.15720 mL	0.14000 mL	2.567	0.00609	0.52065	0.00042	10.0 s
37:06.8	Data point 35	1.50000 mL	0.16729 mL	0.16218 mL	0.14000 mL	2.744	0.00186	0.31955	0.00016	10.0 s
37:52.7	Data point 36	1.50000 mL	0.16729 mL	0.16616 mL	0.14000 mL	2.940	0.00060	0.05168	0.00013	10.5 s

Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
38:28.7	Data point 37	1.50000 mL	0.16729 mL	0.16856 mL	0.14000 mL	3.099	-0.00077	0.04289	0.00018	10.0 s
39:19.8	Data point 38	1.50000 mL	0.16729 mL	0.17136 mL	0.14000 mL	3.295	-0.00378	0.07695	0.00067	10.0 s
40:05.6	Data point 39	1.50000 mL	0.16729 mL	0.17321 mL	0.14000 mL	3.493	-0.00681	0.31042	0.00060	10.5 s
40:46.7	Data point 40	1.50000 mL	0.16729 mL	0.17446 mL	0.14000 mL	3.684	-0.00803	0.18101	0.00093	10.0 s
41:32.4	Data point 41	1.50000 mL	0.16729 mL	0.17561 mL	0.14000 mL	3.965	0.00188	0.07002	0.00035	10.0 s
42:07.9	Data point 42	1.50000 mL	0.16729 mL	0.17655 mL	0.14000 mL	4.455	-0.01704	0.79788	0.00094	10.5 s
42:43.8	Data point 43	1.50000 mL	0.16729 mL	0.17742 mL	0.14000 mL	7.873	-0.08043	0.99747	0.00398	Timed out at 59.5 s
44:14.3	Data point 44	1.50000 mL	0.16729 mL	0.17789 mL	0.14000 mL	9.006	-0.01224	0.48541	0.00087	16.0 s
44:55.8	Data point 45	1.50000 mL	0.16729 mL	0.17862 mL	0.14000 mL	9.515	-0.01874	0.92592	0.00096	11.5 s
45:32.7	Data point 46	1.50000 mL	0.16729 mL	0.17959 mL	0.14000 mL	9.879	-0.00549	0.23712	0.00056	10.0 s
46:18.6	Data point 47	1.50000 mL	0.16729 mL	0.18071 mL	0.14000 mL	10.073	-0.01138	0.44990	0.00084	10.0 s
47:04.3	Data point 48	1.50000 mL	0.16729 mL	0.18187 mL	0.14000 mL	10.258	-0.00900	0.33929	0.00076	10.0 s
47:55.4	Data point 49	1.50000 mL	0.16729 mL	0.18330 mL	0.14000 mL	10.446	-0.00333	0.51756	0.00023	10.0 s
48:30.9	Data point 50	1.50000 mL	0.16729 mL	0.18476 mL	0.14000 mL	10.630	-0.00872	0.81800	0.00048	10.0 s
49:06.3	Data point 51	1.50000 mL	0.16729 mL	0.18648 mL	0.14000 mL	10.779	-0.00578	0.38967	0.00046	10.0 s
49:57.4	Data point 52	1.50000 mL	0.16729 mL	0.18977 mL	0.14000 mL	10.967	0.00098	0.03975	0.00024	10.0 s
50:43.3	Data point 53	1.50000 mL	0.16729 mL	0.19381 mL	0.14000 mL	11.158	-0.00373	0.09690	0.00059	10.0 s
51:34.5	Data point 54	1.50000 mL	0.16729 mL	0.19948 mL	0.14000 mL	11.348	-0.00214	0.18325	0.00025	10.0 s
52:20.5	Data point 55	1.50000 mL	0.16729 mL	0.20715 mL	0.14000 mL	11.543	0.00767	0.67130	0.00046	10.0 s
52:56.2	Data point 56	1.50000 mL	0.16729 mL	0.21816 mL	0.14000 mL	11.723	0.00230	0.01310	0.00099	10.5 s
53:32.6	Data point 57	1.50000 mL	0.16729 mL	0.23492 mL	0.14000 mL	11.912	0.00035	0.00040	0.00087	10.0 s
54:08.4	Data point 58	1.50000 mL	0.16729 mL	0.25125 mL	0.14000 mL	12.032	-0.00066	0.00154	0.00082	10.0 s
55:30.7	Data point 59	1.50000 mL	0.30701 mL	0.25125 mL	0.44000 mL	1.958	-0.01398	0.59830	0.00089	10.5 s
56:17.5	Data point 60	1.50000 mL	0.30701 mL	0.27349 mL	0.44000 mL	2.167	0.01516	0.86723	0.00080	10.5 s
56:53.8	Data point 61	1.50000 mL	0.30701 mL	0.28777 mL	0.44000 mL	2.365	0.00123	0.04714	0.00028	10.0 s
57:29.4	Data point 62	1.50000 mL	0.30701 mL	0.29692 mL	0.44000 mL	2.567	0.00332	0.71527	0.00019	10.0 s
58:05.0	Data point 63	1.50000 mL	0.30701 mL	0.30287 mL	0.44000 mL	2.737	-0.00087	0.02536	0.00027	10.0 s
58:50.9	Data point 64	1.50000 mL	0.30701 mL	0.30748 mL	0.44000 mL	2.936	0.00264	0.18981	0.00030	10.0 s
59:26.4	Data point 65	1.50000 mL	0.30701 mL	0.31054 mL	0.44000 mL	3.144	-0.00133	0.27873	0.00012	10.0 s
1:00:01.9	Data point 66	1.50000 mL	0.30701 mL	0.31298 mL	0.44000 mL	3.378	-0.00152	0.05010	0.00033	10.0 s
1:00:42.5	Data point 67	1.50000 mL	0.30701 mL	0.31430 mL	0.44000 mL	3.580	-0.00279	0.07835	0.00049	10.0 s
1:01:17.9	Data point 68	1.50000 mL	0.30701 mL	0.31538 mL	0.44000 mL	3.878	-0.00524	0.64775	0.00032	10.0 s
1:01:53.4	Data point 69	1.50000 mL	0.30701 mL	0.31642 mL	0.44000 mL	4.674	-0.00689	0.18723	0.00079	12.0 s
1:02:30.8	Data point 70	1.50000 mL	0.30701 mL	0.31686 mL	0.44000 mL	6.215	-0.01858	0.91294	0.00096	51.5 s
1:03:52.9	Data point 71	1.50000 mL	0.30701 mL	0.31724 mL	0.44000 mL	8.470	-0.01798	0.89260	0.00094	50.0 s
1:05:08.4	Data point 72	1.50000 mL	0.30701 mL	0.31740 mL	0.44000 mL	8.775	-0.01405	0.63869	0.00087	14.5 s
1:05:48.3	Data point 73	1.50000 mL	0.30701 mL	0.31771 mL	0.44000 mL	9.175	-0.01421	0.63693	0.00088	12.0 s
1:06:25.7	Data point 74	1.50000 mL	0.30701 mL	0.31834 mL	0.44000 mL	9.635	-0.00550	0.11202	0.00081	10.0 s
1:07:01.2	Data point 75	1.50000 mL	0.30701 mL	0.31933 mL	0.44000 mL	10.000	0.00089	0.00892	0.00046	10.5 s
1:07:37.1	Data point 76	1.50000 mL	0.30701 mL	0.32037 mL	0.44000 mL	10.223	-0.00159	0.02094	0.00054	10.0 s
1:08:23.0	Data point 77	1.50000 mL	0.30701 mL	0.32175 mL	0.44000 mL	10.415	0.00362	0.09900	0.00057	10.0 s
1:09:08.8	Data point 78	1.50000 mL	0.30701 mL	0.32333 mL	0.44000 mL	10.600	0.00093	0.00262	0.00090	10.0 s
1:09:54.6	Data point 79	1.50000 mL	0.30701 mL	0.32545 mL	0.44000 mL	10.784	0.01040	0.85611	0.00056	10.0 s
1:10:30.1	Data point 80	1.50000 mL	0.30701 mL	0.32815 mL	0.44000 mL	10.962	0.00448	0.80191	0.00025	10.0 s
1:11:05.6	Data point 81	1.50000 mL	0.30701 mL	0.33177 mL	0.44000 mL	11.121	0.00570	0.85507	0.00030	10.0 s
1:11:51.6	Data point 82	1.50000 mL	0.30701 mL	0.33711 mL	0.44000 mL	11.309	0.00647	0.21129	0.00070	10.0 s
1:12:27.2	Data point 83	1.50000 mL	0.30701 mL	0.34450 mL	0.44000 mL	11.473	0.00664	0.82184	0.00036	10.0 s
1:13:13.4	Data point 84	1.50000 mL	0.30701 mL	0.35626 mL	0.44000 mL	11.668	0.00657	0.91736	0.00034	10.0 s
1:13:49.2	Data point 85	1.50000 mL	0.30701 mL	0.37333 mL	0.44000 mL	11.850	0.00586	0.31317	0.00052	10.0 s
1:14:25.2	Data point 86	1.50000 mL	0.30701 mL	0.39915 mL	0.44000 mL	12.033	0.00565	0.29376	0.00051	10.0 s
1:14:44.3	Assay volumes	1.50000 mL	0.30701 mL	0.39915 mL	0.44000 mL					

Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
<b>General Settings</b>				
Analyst name	Pion			
<b>Standard Experiment Settings</b>				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
<b>Advanced General Settings</b>				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
<b>Titration Pre-Dose</b>				
Titration pre-dose	None			
<b>Assay Medium</b>				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.040 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
<b>Sample Sonication</b>				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
<b>Sample Dissolution</b>				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
<b>Carbonate purge</b>				
Perform a carbonate purge	No			
<b>Temperature Control</b>				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
<b>Titration 1</b>				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
<b>Titration 2</b>				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			



Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
<b>Titration 3</b>				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.300 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
<b>Data Point Stability</b>				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

## Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	3/1/2018 9:25:33 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	3/1/2018 9:25:33 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	3/1/2018 9:25:33 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	3/1/2018 9:25:33 AM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	3/1/2018 9:25:34 AM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	3/1/2018 9:25:34 AM	C:\Sirius_T3\HCl18B27.t3r

## Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM



Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titration	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titration		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+4.30 mV		3/1/2018 9:26:01 AM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 10:23:32 AM
Wash 2	0.5% Triton X-100 in H2O		2/28/2018 10:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 10:24:06 AM
Buffer position 2	pH 7		2/28/2018 10:24:08 AM
Storage position			2/28/2018 10:21:14 AM
Wash water	8.3e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	7.2e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titration tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name:	<b>M16_octanol</b>	Experiment start time:	<b>3/1/2018 9:25:34 AM</b>
Assay name:	<b>pH-metric high logP</b>	Analyst:	<b>Pion</b>
Assay ID:	<b>18C-01007</b>	Instrument ID:	<b>T312060</b>
Filename:	<b>C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18C-01007_M16_octanol_pH-metric high logP.t3r</b>		

## Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

## Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

## Experiment Log

[2:48] Air gap created for Water (0.15 M KCl)  
 [2:49] Air gap created for Acid (0.5 M HCl)  
 [2:49] Air gap created for Base (0.5 M KOH)  
 [2:49] Air gap released for Water (0.15 M KCl)  
 [2:53] Titrator arm moved over Titration position  
 [2:53] Titration 1 of 3  
 [2:53] Adding initial titrants  
 [2:53] Automatically add 1.50000 mL of water  
 [3:18] Dispensed 1.500000 mL of Water (0.15 M KCl)  
 [3:23] Titrator arm moved over Drain  
 [9:04] Titrator arm moved to Titration position  
 [9:04] Argon flow rate set to 100  
 [9:04] Stirrer speed set to 10  
 [9:09] Automatically add 0.04000 mL of Octanol  
 [9:10] Dispensed 0.040005 mL of Octanol  
 [9:11] Initial pH = 3.56  
 [9:11] Iterative adjust 3.56 -> 2.00  
 [9:11] pH 3.56 -> 2.00  
 [9:13] Air gap released for Acid (0.5 M HCl)  
 [9:14] Dispensed 0.041439 mL of Acid (0.5 M HCl)  
 [9:19] pH 2.01 -> 2.00  
 [9:19] Dispensed 0.001270 mL of Acid (0.5 M HCl)  
 [9:24] Holding pH 2.00  
 [11:24] Stirrer speed set to 0  
 [11:24] Stirrer speed set to 50  
 [11:24] Iterative adjust 1.97 -> 2.00  
 [11:24] pH 1.97 -> 2.00  
 [11:25] Air gap released for Base (0.5 M KOH)  
 [11:26] Dispensed 0.003198 mL of Base (0.5 M KOH)  
 [12:16] Stirrer speed set to 0  
 [12:26] Datapoint id 1 collected  
 [12:26] Stirrer speed set to 50  
 [12:31] pH 2.01 -> 2.21  
 [12:31] Using cautious pH adjust  
 [12:31] Dispensed 0.007714 mL of Base (0.5 M KOH)  
 [12:37] Stepping pH = 2.10  
 [12:37] Dispensed 0.005903 mL of Base (0.5 M KOH)  
 [12:42] Stepping pH = 2.19  
 [12:42] Dispensed 0.000964 mL of Base (0.5 M KOH)  
 [12:47] Stepping pH = 2.21  
 [13:02] Stirrer speed set to 0  
 [13:12] Datapoint id 2 collected

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[13:12] Charge balance equation is out by 5.6%  
[13:12] Stirrer speed set to 50  
[13:17] pH 2.21 -> 2.41  
[13:17] Using charge balance adjust  
[13:18] Dispensed 0.009619 mL of Base (0.5 M KOH)  
[13:38] Stirrer speed set to 0  
[13:48] Datapoint id 3 collected  
[13:48] Charge balance equation is out by -0.3%  
[13:48] Stirrer speed set to 50  
[13:53] pH 2.42 -> 2.62  
[13:53] Using charge balance adjust  
[13:53] Dispensed 0.005997 mL of Base (0.5 M KOH)  
[14:13] Stirrer speed set to 0  
[14:23] Datapoint id 4 collected  
[14:23] Charge balance equation is out by -11.6%  
[14:23] Stirrer speed set to 50  
[14:29] pH 2.60 -> 2.80  
[14:29] Using charge balance adjust  
[14:29] Dispensed 0.003975 mL of Base (0.5 M KOH)  
[14:49] Stirrer speed set to 0  
[14:59] Datapoint id 5 collected  
[14:59] Charge balance equation is out by -5.5%  
[14:59] Stirrer speed set to 50  
[15:04] pH 2.80 -> 3.00  
[15:04] Using charge balance adjust  
[15:04] Dispensed 0.002611 mL of Base (0.5 M KOH)  
[15:24] Stirrer speed set to 0  
[15:34] Datapoint id 6 collected  
[15:34] Charge balance equation is out by -31.1%  
[15:34] Stirrer speed set to 50  
[15:40] pH 2.94 -> 3.14  
[15:40] Using cautious pH adjust  
[15:40] Dispensed 0.000988 mL of Base (0.5 M KOH)  
[15:45] Stepping pH = 3.01  
[15:45] Dispensed 0.001152 mL of Base (0.5 M KOH)  
[15:50] Stepping pH = 3.09  
[15:50] Dispensed 0.000494 mL of Base (0.5 M KOH)  
[15:55] Stepping pH = 3.13  
[16:10] Stirrer speed set to 0  
[16:20] Datapoint id 7 collected  
[16:20] Charge balance equation is out by -33.7%  
[16:20] Stirrer speed set to 50  
[16:25] pH 3.14 -> 3.34  
[16:25] Using cautious pH adjust  
[16:25] Dispensed 0.000729 mL of Base (0.5 M KOH)  
[16:31] Stepping pH = 3.20  
[16:31] Dispensed 0.000823 mL of Base (0.5 M KOH)  
[16:36] Stepping pH = 3.28  
[16:36] Dispensed 0.000400 mL of Base (0.5 M KOH)  
[16:41] Stepping pH = 3.32  
[16:41] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[16:46] Stepping pH = 3.33  
[17:01] Stirrer speed set to 0  
[17:11] Datapoint id 8 collected  
[17:11] Charge balance equation is out by -44.8%  
[17:11] Stirrer speed set to 50  
[17:16] pH 3.33 -> 3.53  
[17:16] Using cautious pH adjust  
[17:16] Dispensed 0.000588 mL of Base (0.5 M KOH)

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[17:22] Stepping pH = 3.39  
[17:22] Dispensed 0.000729 mL of Base (0.5 M KOH)  
[17:27] Stepping pH = 3.46  
[17:27] Dispensed 0.000447 mL of Base (0.5 M KOH)  
[17:32] Stepping pH = 3.51  
[17:32] Dispensed 0.000188 mL of Base (0.5 M KOH)  
[17:37] Stepping pH = 3.52  
[17:52] Stirrer speed set to 0  
[18:02] Datapoint id 9 collected  
[18:02] Charge balance equation is out by -64.9%  
[18:02] Stirrer speed set to 50  
[18:07] pH 3.52 -> 3.72  
[18:07] Using cautious pH adjust  
[18:07] Dispensed 0.000564 mL of Base (0.5 M KOH)  
[18:13] Stepping pH = 3.58  
[18:13] Dispensed 0.000706 mL of Base (0.5 M KOH)  
[18:18] Stepping pH = 3.64  
[18:18] Dispensed 0.000564 mL of Base (0.5 M KOH)  
[18:23] Stepping pH = 3.71  
[18:23] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[18:28] Stepping pH = 3.71  
[18:43] Stirrer speed set to 0  
[18:53] Datapoint id 10 collected  
[18:53] Charge balance equation is out by -71.8%  
[18:53] Stirrer speed set to 50  
[18:58] pH 3.71 -> 3.91  
[18:58] Using cautious pH adjust  
[18:58] Dispensed 0.000611 mL of Base (0.5 M KOH)  
[19:03] Stepping pH = 3.79  
[19:04] Dispensed 0.000588 mL of Base (0.5 M KOH)  
[19:09] Stepping pH = 3.87  
[19:09] Dispensed 0.000259 mL of Base (0.5 M KOH)  
[19:14] Stepping pH = 3.90  
[19:14] Dispensed 0.000094 mL of Base (0.5 M KOH)  
[19:19] Stepping pH = 3.91  
[19:34] Stirrer speed set to 0  
[19:44] Datapoint id 11 collected  
[19:44] Charge balance equation is out by -28.6%  
[19:44] Stirrer speed set to 50  
[19:49] pH 3.91 -> 4.11  
[19:49] Using cautious pH adjust  
[19:49] Dispensed 0.000706 mL of Base (0.5 M KOH)  
[19:54] Stepping pH = 4.05  
[19:55] Dispensed 0.000282 mL of Base (0.5 M KOH)  
[20:00] Stepping pH = 4.10  
[20:15] Stirrer speed set to 0  
[20:25] Datapoint id 12 collected  
[20:25] Charge balance equation is out by 30.4%  
[20:25] Stirrer speed set to 50  
[20:30] pH 4.10 -> 4.30  
[20:30] Using cautious pH adjust  
[20:30] Dispensed 0.000823 mL of Base (0.5 M KOH)  
[20:35] Stepping pH = 4.37  
[20:50] Stirrer speed set to 0  
[21:01] Datapoint id 13 collected  
[21:01] Charge balance equation is out by 50.0%  
[21:01] Stirrer speed set to 50  
[21:06] pH 4.36 -> 4.56  
[21:06] Using cautious pH adjust

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[21:06] Dispensed 0.000917 mL of Base (0.5 M KOH)  
[21:11] Stepping pH = 4.99  
[21:26] Stirrer speed set to 0  
[21:39] Datapoint id 14 collected  
[21:39] Charge balance equation is out by 50.0%  
[21:39] Stirrer speed set to 50  
[21:44] pH 4.97 -> 5.17  
[21:44] Using cautious pH adjust  
[21:44] Dispensed 0.000682 mL of Base (0.5 M KOH)  
[21:49] Stepping pH = 8.17  
[22:05] Stirrer speed set to 0  
[22:39] Datapoint id 15 collected  
[22:39] Charge balance equation is out by 50.0%  
[22:39] Stirrer speed set to 50  
[22:44] pH 8.55 -> 8.75  
[22:44] Using cautious pH adjust  
[22:44] Dispensed 0.000564 mL of Base (0.5 M KOH)  
[22:49] Stepping pH = 9.23  
[23:04] Stirrer speed set to 0  
[23:19] Datapoint id 16 collected  
[23:19] Charge balance equation is out by 50.0%  
[23:19] Stirrer speed set to 50  
[23:24] pH 9.22 -> 9.42  
[23:24] Using cautious pH adjust  
[23:24] Dispensed 0.000941 mL of Base (0.5 M KOH)  
[23:29] Stepping pH = 9.65  
[23:44] Stirrer speed set to 0  
[23:54] Datapoint id 17 collected  
[23:54] Charge balance equation is out by 50.0%  
[23:54] Stirrer speed set to 50  
[24:00] pH 9.63 -> 9.83  
[24:00] Using cautious pH adjust  
[24:00] Dispensed 0.000776 mL of Base (0.5 M KOH)  
[24:05] Stepping pH = 9.82  
[24:05] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[24:10] Stepping pH = 9.82  
[24:10] Dispensed 0.000259 mL of Base (0.5 M KOH)  
[24:15] Stepping pH = 9.88  
[24:30] Stirrer speed set to 0  
[24:41] Datapoint id 18 collected  
[24:41] Charge balance equation is out by 30.2%  
[24:41] Stirrer speed set to 50  
[24:46] pH 9.87 -> 10.07  
[24:46] Using cautious pH adjust  
[24:46] Dispensed 0.000635 mL of Base (0.5 M KOH)  
[24:51] Stepping pH = 9.99  
[24:51] Dispensed 0.000282 mL of Base (0.5 M KOH)  
[24:56] Stepping pH = 10.02  
[24:56] Dispensed 0.000235 mL of Base (0.5 M KOH)  
[25:02] Stepping pH = 10.06  
[25:17] Stirrer speed set to 0  
[25:27] Datapoint id 19 collected  
[25:27] Charge balance equation is out by 7.6%  
[25:27] Stirrer speed set to 50  
[25:32] pH 10.05 -> 10.25  
[25:32] Using charge balance adjust  
[25:32] Dispensed 0.001082 mL of Base (0.5 M KOH)  
[25:52] Stirrer speed set to 0  
[26:02] Datapoint id 20 collected

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[26:02] Charge balance equation is out by -29.3%  
[26:02] Stirrer speed set to 50  
[26:07] pH 10.19 -> 10.39  
[26:07] Using cautious pH adjust  
[26:07] Dispensed 0.000517 mL of Base (0.5 M KOH)  
[26:12] Stepping pH = 10.25  
[26:12] Dispensed 0.000635 mL of Base (0.5 M KOH)  
[26:18] Stepping pH = 10.34  
[26:18] Dispensed 0.000329 mL of Base (0.5 M KOH)  
[26:23] Stepping pH = 10.37  
[26:23] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[26:28] Stepping pH = 10.39  
[26:43] Stirrer speed set to 0  
[26:53] Datapoint id 21 collected  
[26:53] Charge balance equation is out by -61.1%  
[26:53] Stirrer speed set to 50  
[26:58] pH 10.38 -> 10.58  
[26:58] Using cautious pH adjust  
[26:58] Dispensed 0.000517 mL of Base (0.5 M KOH)  
[27:03] Stepping pH = 10.45  
[27:03] Dispensed 0.000611 mL of Base (0.5 M KOH)  
[27:08] Stepping pH = 10.52  
[27:08] Dispensed 0.000353 mL of Base (0.5 M KOH)  
[27:14] Stepping pH = 10.56  
[27:14] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[27:19] Stepping pH = 10.58  
[27:34] Stirrer speed set to 0  
[27:44] Datapoint id 22 collected  
[27:44] Charge balance equation is out by -57.1%  
[27:44] Stirrer speed set to 50  
[27:49] pH 10.57 -> 10.77  
[27:49] Using cautious pH adjust  
[27:49] Dispensed 0.000611 mL of Base (0.5 M KOH)  
[27:54] Stepping pH = 10.64  
[27:54] Dispensed 0.000706 mL of Base (0.5 M KOH)  
[27:59] Stepping pH = 10.72  
[28:00] Dispensed 0.000400 mL of Base (0.5 M KOH)  
[28:05] Stepping pH = 10.75  
[28:05] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[28:10] Stepping pH = 10.76  
[28:25] Stirrer speed set to 0  
[28:35] Datapoint id 23 collected  
[28:35] Charge balance equation is out by -50.4%  
[28:35] Stirrer speed set to 50  
[28:40] pH 10.75 -> 10.95  
[28:40] Using cautious pH adjust  
[28:40] Dispensed 0.000823 mL of Base (0.5 M KOH)  
[28:45] Stepping pH = 10.83  
[28:45] Dispensed 0.000941 mL of Base (0.5 M KOH)  
[28:50] Stepping pH = 10.90  
[28:51] Dispensed 0.000588 mL of Base (0.5 M KOH)  
[28:56] Stepping pH = 10.94  
[28:56] Dispensed 0.000212 mL of Base (0.5 M KOH)  
[29:01] Stepping pH = 10.94  
[29:16] Stirrer speed set to 0  
[29:26] Datapoint id 24 collected  
[29:26] Charge balance equation is out by -55.0%  
[29:26] Stirrer speed set to 50  
[29:31] pH 10.94 -> 11.14



Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[29:31] Using cautious pH adjust  
[29:31] Dispensed 0.001199 mL of Base (0.5 M KOH)  
[29:36] Stepping pH = 11.01  
[29:36] Dispensed 0.001458 mL of Base (0.5 M KOH)  
[29:42] Stepping pH = 11.09  
[29:42] Dispensed 0.000706 mL of Base (0.5 M KOH)  
[29:47] Stepping pH = 11.13  
[29:47] Dispensed 0.000188 mL of Base (0.5 M KOH)  
[29:52] Stepping pH = 11.14  
[30:07] Stirrer speed set to 0  
[30:17] Datapoint id 25 collected  
[30:17] Charge balance equation is out by -48.0%  
[30:17] Stirrer speed set to 50  
[30:22] pH 11.13 -> 11.33  
[30:22] Using cautious pH adjust  
[30:22] Dispensed 0.001787 mL of Base (0.5 M KOH)  
[30:27] Stepping pH = 11.22  
[30:28] Dispensed 0.001552 mL of Base (0.5 M KOH)  
[30:33] Stepping pH = 11.30  
[30:33] Dispensed 0.000611 mL of Base (0.5 M KOH)  
[30:38] Stepping pH = 11.32  
[30:53] Stirrer speed set to 0  
[31:03] Datapoint id 26 collected  
[31:03] Charge balance equation is out by -10.0%  
[31:03] Stirrer speed set to 50  
[31:08] pH 11.32 -> 11.52  
[31:08] Using charge balance adjust  
[31:08] Dispensed 0.005503 mL of Base (0.5 M KOH)  
[31:29] Stirrer speed set to 0  
[31:39] Datapoint id 27 collected  
[31:39] Charge balance equation is out by -14.2%  
[31:39] Stirrer speed set to 50  
[31:44] pH 11.49 -> 11.69  
[31:44] Using charge balance adjust  
[31:44] Dispensed 0.008278 mL of Base (0.5 M KOH)  
[32:04] Stirrer speed set to 0  
[32:14] Datapoint id 28 collected  
[32:14] Charge balance equation is out by -7.1%  
[32:14] Stirrer speed set to 50  
[32:19] pH 11.68 -> 11.88  
[32:19] Using charge balance adjust  
[32:20] Dispensed 0.013006 mL of Base (0.5 M KOH)  
[32:40] Stirrer speed set to 0  
[32:50] Datapoint id 29 collected  
[32:50] Charge balance equation is out by -8.7%  
[32:50] Stirrer speed set to 50  
[32:55] pH 11.87 -> 12.05  
[32:55] Using charge balance adjust  
[32:56] Dispensed 0.017803 mL of Base (0.5 M KOH)  
[33:16] Stirrer speed set to 0  
[33:26] Datapoint id 30 collected  
[33:26] Charge balance equation is out by -21.5%  
[33:26] Titration 2 of 3  
[33:26] Adding initial titrants  
[33:26] Automatically add 0.10000 mL of Octanol  
[33:28] Dispensed 0.100000 mL of Octanol  
[33:28] Stirrer speed set to 10  
[33:29] Stirrer speed set to 55  
[33:29] Iterative adjust 12.04 -> 2.00

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[33:29] pH 12.04 -> 2.00  
[33:32] Dispensed 0.100000 mL of Acid (0.5 M HCl)  
[33:37] pH 2.26 -> 2.00  
[33:38] Dispensed 0.022437 mL of Acid (0.5 M HCl)  
[33:43] pH 2.02 -> 2.00  
[33:43] Dispensed 0.002140 mL of Acid (0.5 M HCl)  
[34:33] Stirrer speed set to 0  
[34:43] Datapoint id 31 collected  
[34:43] Stirrer speed set to 55  
[34:48] pH 1.96 -> 2.16  
[34:48] Using cautious pH adjust  
[34:49] Dispensed 0.010113 mL of Base (0.5 M KOH)  
[34:54] Stepping pH = 2.06  
[34:54] Dispensed 0.006703 mL of Base (0.5 M KOH)  
[34:59] Stepping pH = 2.13  
[34:59] Dispensed 0.002070 mL of Base (0.5 M KOH)  
[35:04] Stepping pH = 2.16  
[35:19] Stirrer speed set to 0  
[35:30] Datapoint id 32 collected  
[35:30] Charge balance equation is out by 6.7%  
[35:30] Stirrer speed set to 55  
[35:35] pH 2.16 -> 2.36  
[35:35] Using charge balance adjust  
[35:35] Dispensed 0.012629 mL of Base (0.5 M KOH)  
[35:55] Stirrer speed set to 0  
[36:05] Datapoint id 33 collected  
[36:05] Charge balance equation is out by 11.2%  
[36:05] Stirrer speed set to 55  
[36:10] pH 2.39 -> 2.59  
[36:10] Using charge balance adjust  
[36:11] Dispensed 0.007479 mL of Base (0.5 M KOH)  
[36:31] Stirrer speed set to 0  
[36:41] Datapoint id 34 collected  
[36:41] Charge balance equation is out by -11.6%  
[36:41] Stirrer speed set to 55  
[36:46] pH 2.57 -> 2.77  
[36:46] Using charge balance adjust  
[36:46] Dispensed 0.004986 mL of Base (0.5 M KOH)  
[37:06] Stirrer speed set to 0  
[37:16] Datapoint id 35 collected  
[37:16] Charge balance equation is out by -15.2%  
[37:16] Stirrer speed set to 55  
[37:21] pH 2.75 -> 2.95  
[37:21] Using cautious pH adjust  
[37:22] Dispensed 0.001740 mL of Base (0.5 M KOH)  
[37:27] Stepping pH = 2.82  
[37:27] Dispensed 0.001740 mL of Base (0.5 M KOH)  
[37:32] Stepping pH = 2.91  
[37:32] Dispensed 0.000494 mL of Base (0.5 M KOH)  
[37:37] Stepping pH = 2.94  
[37:52] Stirrer speed set to 0  
[38:03] Datapoint id 36 collected  
[38:03] Charge balance equation is out by -14.7%  
[38:03] Stirrer speed set to 55  
[38:08] pH 2.94 -> 3.14  
[38:08] Using charge balance adjust  
[38:08] Dispensed 0.002399 mL of Base (0.5 M KOH)  
[38:28] Stirrer speed set to 0  
[38:38] Datapoint id 37 collected



Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[38:38] Charge balance equation is out by -22.9%  
[38:38] Stirrer speed set to 55  
[38:43] pH 3.10 -> 3.30  
[38:43] Using cautious pH adjust  
[38:44] Dispensed 0.000941 mL of Base (0.5 M KOH)  
[38:49] Stepping pH = 3.17  
[38:49] Dispensed 0.001105 mL of Base (0.5 M KOH)  
[38:54] Stepping pH = 3.25  
[38:54] Dispensed 0.000611 mL of Base (0.5 M KOH)  
[38:59] Stepping pH = 3.29  
[38:59] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[39:04] Stepping pH = 3.30  
[39:19] Stirrer speed set to 0  
[39:29] Datapoint id 38 collected  
[39:29] Charge balance equation is out by -46.9%  
[39:29] Stirrer speed set to 55  
[39:34] pH 3.30 -> 3.50  
[39:34] Using cautious pH adjust  
[39:35] Dispensed 0.000800 mL of Base (0.5 M KOH)  
[39:40] Stepping pH = 3.38  
[39:40] Dispensed 0.000776 mL of Base (0.5 M KOH)  
[39:45] Stepping pH = 3.46  
[39:45] Dispensed 0.000282 mL of Base (0.5 M KOH)  
[39:50] Stepping pH = 3.50  
[40:05] Stirrer speed set to 0  
[40:16] Datapoint id 39 collected  
[40:16] Charge balance equation is out by -15.2%  
[40:16] Stirrer speed set to 55  
[40:21] pH 3.50 -> 3.70  
[40:21] Using cautious pH adjust  
[40:21] Dispensed 0.000776 mL of Base (0.5 M KOH)  
[40:26] Stepping pH = 3.61  
[40:26] Dispensed 0.000470 mL of Base (0.5 M KOH)  
[40:31] Stepping pH = 3.69  
[40:46] Stirrer speed set to 0  
[40:56] Datapoint id 40 collected  
[40:56] Charge balance equation is out by 19.5%  
[40:56] Stirrer speed set to 55  
[41:01] pH 3.69 -> 3.89  
[41:01] Using cautious pH adjust  
[41:02] Dispensed 0.000823 mL of Base (0.5 M KOH)  
[41:07] Stepping pH = 3.88  
[41:07] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[41:12] Stepping pH = 3.88  
[41:12] Dispensed 0.000282 mL of Base (0.5 M KOH)  
[41:17] Stepping pH = 3.96  
[41:32] Stirrer speed set to 0  
[41:42] Datapoint id 41 collected  
[41:42] Charge balance equation is out by 29.0%  
[41:42] Stirrer speed set to 55  
[41:47] pH 3.97 -> 4.17  
[41:47] Using cautious pH adjust  
[41:47] Dispensed 0.000941 mL of Base (0.5 M KOH)  
[41:52] Stepping pH = 4.46  
[42:07] Stirrer speed set to 0  
[42:18] Datapoint id 42 collected  
[42:18] Charge balance equation is out by 50.0%  
[42:18] Stirrer speed set to 55  
[42:23] pH 4.46 -> 4.66

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[42:23] Using cautious pH adjust  
[42:23] Dispensed 0.000870 mL of Base (0.5 M KOH)  
[42:28] Stepping pH = 7.47  
[42:43] Stirrer speed set to 0  
[43:43] Datapoint id 43 collected  
[43:43] Charge balance equation is out by 50.0%  
[43:43] Stirrer speed set to 55  
[43:48] pH 7.65 -> 7.85  
[43:48] Using cautious pH adjust  
[43:49] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[43:54] Stepping pH = 7.58  
[43:54] Dispensed 0.000400 mL of Base (0.5 M KOH)  
[43:59] Stepping pH = 9.04  
[44:14] Stirrer speed set to 0  
[44:30] Datapoint id 44 collected  
[44:30] Charge balance equation is out by -270.4%  
[44:30] Stirrer speed set to 55  
[44:35] pH 9.00 -> 9.20  
[44:35] Using cautious pH adjust  
[44:35] Dispensed 0.000729 mL of Base (0.5 M KOH)  
[44:40] Stepping pH = 9.52  
[44:55] Stirrer speed set to 0  
[45:07] Datapoint id 45 collected  
[45:07] Charge balance equation is out by 50.0%  
[45:07] Stirrer speed set to 55  
[45:12] pH 9.51 -> 9.71  
[45:12] Using cautious pH adjust  
[45:12] Dispensed 0.000964 mL of Base (0.5 M KOH)  
[45:17] Stepping pH = 9.88  
[45:32] Stirrer speed set to 0  
[45:42] Datapoint id 46 collected  
[45:42] Charge balance equation is out by 50.0%  
[45:42] Stirrer speed set to 55  
[45:47] pH 9.88 -> 10.08  
[45:47] Using cautious pH adjust  
[45:48] Dispensed 0.000847 mL of Base (0.5 M KOH)  
[45:53] Stepping pH = 10.05  
[45:53] Dispensed 0.000118 mL of Base (0.5 M KOH)  
[45:58] Stepping pH = 10.06  
[45:58] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[46:03] Stepping pH = 10.08  
[46:18] Stirrer speed set to 0  
[46:28] Datapoint id 47 collected  
[46:28] Charge balance equation is out by 32.6%  
[46:28] Stirrer speed set to 55  
[46:33] pH 10.08 -> 10.28  
[46:33] Using cautious pH adjust  
[46:33] Dispensed 0.000753 mL of Base (0.5 M KOH)  
[46:38] Stepping pH = 10.22  
[46:39] Dispensed 0.000259 mL of Base (0.5 M KOH)  
[46:44] Stepping pH = 10.25  
[46:44] Dispensed 0.000141 mL of Base (0.5 M KOH)  
[46:49] Stepping pH = 10.27  
[47:04] Stirrer speed set to 0  
[47:14] Datapoint id 48 collected  
[47:14] Charge balance equation is out by 22.5%  
[47:14] Stirrer speed set to 55  
[47:19] pH 10.26 -> 10.46  
[47:19] Using cautious pH adjust

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[47:19] Dispensed 0.000706 mL of Base (0.5 M KOH)  
[47:24] Stepping pH = 10.37  
[47:24] Dispensed 0.000423 mL of Base (0.5 M KOH)  
[47:29] Stepping pH = 10.43  
[47:30] Dispensed 0.000235 mL of Base (0.5 M KOH)  
[47:35] Stepping pH = 10.45  
[47:35] Dispensed 0.000071 mL of Base (0.5 M KOH)  
[47:40] Stepping pH = 10.45  
[47:55] Stirrer speed set to 0  
[48:05] Datapoint id 49 collected  
[48:05] Charge balance equation is out by -1.7%  
[48:05] Stirrer speed set to 55  
[48:10] pH 10.45 -> 10.65  
[48:10] Using charge balance adjust  
[48:10] Dispensed 0.001458 mL of Base (0.5 M KOH)  
[48:30] Stirrer speed set to 0  
[48:40] Datapoint id 50 collected  
[48:40] Charge balance equation is out by -9.7%  
[48:40] Stirrer speed set to 55  
[48:46] pH 10.63 -> 10.83  
[48:46] Using charge balance adjust  
[48:46] Dispensed 0.001717 mL of Base (0.5 M KOH)  
[49:06] Stirrer speed set to 0  
[49:16] Datapoint id 51 collected  
[49:16] Charge balance equation is out by -26.7%  
[49:16] Stirrer speed set to 55  
[49:21] pH 10.78 -> 10.98  
[49:21] Using cautious pH adjust  
[49:21] Dispensed 0.001058 mL of Base (0.5 M KOH)  
[49:26] Stepping pH = 10.85  
[49:26] Dispensed 0.001199 mL of Base (0.5 M KOH)  
[49:31] Stepping pH = 10.92  
[49:32] Dispensed 0.000753 mL of Base (0.5 M KOH)  
[49:37] Stepping pH = 10.96  
[49:37] Dispensed 0.000282 mL of Base (0.5 M KOH)  
[49:42] Stepping pH = 10.97  
[49:57] Stirrer speed set to 0  
[50:07] Datapoint id 52 collected  
[50:07] Charge balance equation is out by -54.7%  
[50:07] Stirrer speed set to 55  
[50:12] pH 10.97 -> 11.17  
[50:12] Using cautious pH adjust  
[50:12] Dispensed 0.001529 mL of Base (0.5 M KOH)  
[50:17] Stepping pH = 11.05  
[50:18] Dispensed 0.001646 mL of Base (0.5 M KOH)  
[50:23] Stepping pH = 11.13  
[50:23] Dispensed 0.000870 mL of Base (0.5 M KOH)  
[50:28] Stepping pH = 11.16  
[50:43] Stirrer speed set to 0  
[50:53] Datapoint id 53 collected  
[50:53] Charge balance equation is out by -31.7%  
[50:53] Stirrer speed set to 55  
[50:58] pH 11.16 -> 11.36  
[50:58] Using cautious pH adjust  
[50:58] Dispensed 0.002258 mL of Base (0.5 M KOH)  
[51:03] Stepping pH = 11.25  
[51:03] Dispensed 0.001929 mL of Base (0.5 M KOH)  
[51:09] Stepping pH = 11.32  
[51:09] Dispensed 0.001152 mL of Base (0.5 M KOH)

Sample name: **M16\_octanol**  
 Assay name: **pH-metric high logP**  
 Assay ID: **18C-01007**  
 Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
 Analyst: **Pion**  
 Instrument ID: **T312060**

## Experiment Log (continued)

[51:14] Stepping pH = 11.35  
 [51:14] Dispensed 0.000329 mL of Base (0.5 M KOH)  
 [51:19] Stepping pH = 11.36  
 [51:34] Stirrer speed set to 0  
 [51:44] Datapoint id 54 collected  
 [51:44] Charge balance equation is out by -25.3%  
 [51:44] Stirrer speed set to 55  
 [51:49] pH 11.35 -> 11.55  
 [51:49] Using cautious pH adjust  
 [51:49] Dispensed 0.003504 mL of Base (0.5 M KOH)  
 [51:54] Stepping pH = 11.45  
 [51:55] Dispensed 0.002987 mL of Base (0.5 M KOH)  
 [52:00] Stepping pH = 11.52  
 [52:00] Dispensed 0.001176 mL of Base (0.5 M KOH)  
 [52:05] Stepping pH = 11.55  
 [52:20] Stirrer speed set to 0  
 [52:30] Datapoint id 55 collected  
 [52:30] Charge balance equation is out by -9.2%  
 [52:30] Stirrer speed set to 55  
 [52:35] pH 11.55 -> 11.75  
 [52:35] Using charge balance adjust  
 [52:36] Dispensed 0.011007 mL of Base (0.5 M KOH)  
 [52:56] Stirrer speed set to 0  
 [53:06] Datapoint id 56 collected  
 [53:06] Charge balance equation is out by -12.5%  
 [53:06] Stirrer speed set to 55  
 [53:11] pH 11.73 -> 11.93  
 [53:11] Using charge balance adjust  
 [53:12] Dispensed 0.016769 mL of Base (0.5 M KOH)  
 [53:32] Stirrer speed set to 0  
 [53:42] Datapoint id 57 collected  
 [53:42] Charge balance equation is out by -8.0%  
 [53:42] Stirrer speed set to 55  
 [53:47] pH 11.92 -> 12.05  
 [53:47] Using charge balance adjust  
 [53:48] Dispensed 0.016322 mL of Base (0.5 M KOH)  
 [54:08] Stirrer speed set to 0  
 [54:18] Datapoint id 58 collected  
 [54:18] Charge balance equation is out by -42.2%  
 [54:18] Titration 3 of 3  
 [54:18] Adding initial titrants  
 [54:18] Automatically add 0.30000 mL of Octanol  
 [54:25] Dispensed 0.300000 mL of Octanol  
 [54:25] Stirrer speed set to 10  
 [54:26] Stirrer speed set to 60  
 [54:26] Iterative adjust 12.04 -> 2.00  
 [54:26] pH 12.04 -> 2.00  
 [54:29] Dispensed 0.100000 mL of Acid (0.5 M HCl)  
 [54:34] pH 2.44 -> 2.00  
 [54:35] Dispensed 0.035842 mL of Acid (0.5 M HCl)  
 [54:40] pH 2.03 -> 2.00  
 [54:40] Dispensed 0.003881 mL of Acid (0.5 M HCl)  
 [55:30] Stirrer speed set to 0  
 [55:41] Datapoint id 59 collected  
 [55:41] Stirrer speed set to 60  
 [55:46] pH 1.97 -> 2.17  
 [55:46] Using cautious pH adjust  
 [55:46] Dispensed 0.011477 mL of Base (0.5 M KOH)  
 [55:51] Stepping pH = 2.05

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[55:52] Dispensed 0.008937 mL of Base (0.5 M KOH)  
[55:57] Stepping pH = 2.14  
[55:57] Dispensed 0.001834 mL of Base (0.5 M KOH)  
[56:02] Stepping pH = 2.17  
[56:17] Stirrer speed set to 0  
[56:28] Datapoint id 60 collected  
[56:28] Charge balance equation is out by 3.1%  
[56:28] Stirrer speed set to 60  
[56:33] pH 2.17 -> 2.37  
[56:33] Using charge balance adjust  
[56:33] Dispensed 0.014276 mL of Base (0.5 M KOH)  
[56:53] Stirrer speed set to 0  
[57:03] Datapoint id 61 collected  
[57:03] Charge balance equation is out by -3.3%  
[57:03] Stirrer speed set to 60  
[57:08] pH 2.37 -> 2.57  
[57:08] Using charge balance adjust  
[57:09] Dispensed 0.009149 mL of Base (0.5 M KOH)  
[57:29] Stirrer speed set to 0  
[57:39] Datapoint id 62 collected  
[57:39] Charge balance equation is out by -1.3%  
[57:39] Stirrer speed set to 60  
[57:44] pH 2.57 -> 2.77  
[57:44] Using charge balance adjust  
[57:44] Dispensed 0.005950 mL of Base (0.5 M KOH)  
[58:05] Stirrer speed set to 0  
[58:15] Datapoint id 63 collected  
[58:15] Charge balance equation is out by -16.5%  
[58:15] Stirrer speed set to 60  
[58:20] pH 2.74 -> 2.94  
[58:20] Using cautious pH adjust  
[58:20] Dispensed 0.002117 mL of Base (0.5 M KOH)  
[58:25] Stepping pH = 2.82  
[58:25] Dispensed 0.001952 mL of Base (0.5 M KOH)  
[58:30] Stepping pH = 2.91  
[58:30] Dispensed 0.000541 mL of Base (0.5 M KOH)  
[58:35] Stepping pH = 2.94  
[58:50] Stirrer speed set to 0  
[59:00] Datapoint id 64 collected  
[59:00] Charge balance equation is out by -8.5%  
[59:00] Stirrer speed set to 60  
[59:06] pH 2.94 -> 3.14  
[59:06] Using charge balance adjust  
[59:06] Dispensed 0.003057 mL of Base (0.5 M KOH)  
[59:26] Stirrer speed set to 0  
[59:36] Datapoint id 65 collected  
[59:36] Charge balance equation is out by 2.6%  
[59:36] Stirrer speed set to 60  
[59:41] pH 3.15 -> 3.35  
[59:41] Using charge balance adjust  
[59:41] Dispensed 0.002446 mL of Base (0.5 M KOH)  
[1:00:01] Stirrer speed set to 0  
[1:00:11] Datapoint id 66 collected  
[1:00:11] Charge balance equation is out by 15.7%  
[1:00:11] Stirrer speed set to 60  
[1:00:17] pH 3.38 -> 3.58  
[1:00:17] Using cautious pH adjust  
[1:00:17] Dispensed 0.001105 mL of Base (0.5 M KOH)  
[1:00:22] Stepping pH = 3.54

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:00:22] Dispensed 0.000212 mL of Base (0.5 M KOH)  
[1:00:27] Stepping pH = 3.58  
[1:00:42] Stirrer speed set to 0  
[1:00:52] Datapoint id 67 collected  
[1:00:52] Charge balance equation is out by 40.2%  
[1:00:52] Stirrer speed set to 60  
[1:00:57] pH 3.58 -> 3.78  
[1:00:57] Using cautious pH adjust  
[1:00:57] Dispensed 0.001082 mL of Base (0.5 M KOH)  
[1:01:02] Stepping pH = 3.88  
[1:01:18] Stirrer speed set to 0  
[1:01:28] Datapoint id 68 collected  
[1:01:28] Charge balance equation is out by 50.0%  
[1:01:28] Stirrer speed set to 60  
[1:01:33] pH 3.88 -> 4.08  
[1:01:33] Using cautious pH adjust  
[1:01:33] Dispensed 0.001035 mL of Base (0.5 M KOH)  
[1:01:38] Stepping pH = 4.71  
[1:01:53] Stirrer speed set to 0  
[1:02:05] Datapoint id 69 collected  
[1:02:05] Charge balance equation is out by 50.0%  
[1:02:05] Stirrer speed set to 60  
[1:02:10] pH 4.69 -> 4.89  
[1:02:10] Using cautious pH adjust  
[1:02:10] Dispensed 0.000447 mL of Base (0.5 M KOH)  
[1:02:15] Stepping pH = 6.55  
[1:02:30] Stirrer speed set to 0  
[1:03:22] Datapoint id 70 collected  
[1:03:22] Charge balance equation is out by 50.0%  
[1:03:22] Stirrer speed set to 60  
[1:03:27] pH 6.17 -> 6.37  
[1:03:27] Using cautious pH adjust  
[1:03:27] Dispensed 0.000047 mL of Base (0.5 M KOH)  
[1:03:32] Stepping pH = 6.09  
[1:03:32] Dispensed 0.000329 mL of Base (0.5 M KOH)  
[1:03:37] Stepping pH = 8.68  
[1:03:52] Stirrer speed set to 0  
[1:04:43] Datapoint id 71 collected  
[1:04:43] Charge balance equation is out by -318.8%  
[1:04:43] Stirrer speed set to 60  
[1:04:48] pH 8.44 -> 8.64  
[1:04:48] Using cautious pH adjust  
[1:04:48] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[1:04:53] Stepping pH = 8.82  
[1:05:08] Stirrer speed set to 0  
[1:05:22] Datapoint id 72 collected  
[1:05:22] Charge balance equation is out by 50.0%  
[1:05:22] Stirrer speed set to 60  
[1:05:28] pH 8.77 -> 8.97  
[1:05:28] Using cautious pH adjust  
[1:05:28] Dispensed 0.000306 mL of Base (0.5 M KOH)  
[1:05:33] Stepping pH = 9.20  
[1:05:48] Stirrer speed set to 0  
[1:06:00] Datapoint id 73 collected  
[1:06:00] Charge balance equation is out by 50.0%  
[1:06:00] Stirrer speed set to 60  
[1:06:05] pH 9.18 -> 9.38  
[1:06:05] Using cautious pH adjust  
[1:06:05] Dispensed 0.000635 mL of Base (0.5 M KOH)



Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:06:10] Stepping pH = 9.65  
[1:06:25] Stirrer speed set to 0  
[1:06:35] Datapoint id 74 collected  
[1:06:35] Charge balance equation is out by 50.0%  
[1:06:35] Stirrer speed set to 60  
[1:06:40] pH 9.64 -> 9.84  
[1:06:40] Using cautious pH adjust  
[1:06:41] Dispensed 0.000988 mL of Base (0.5 M KOH)  
[1:06:46] Stepping pH = 10.01  
[1:07:01] Stirrer speed set to 0  
[1:07:11] Datapoint id 75 collected  
[1:07:11] Charge balance equation is out by 50.0%  
[1:07:11] Stirrer speed set to 60  
[1:07:16] pH 10.00 -> 10.20  
[1:07:16] Using cautious pH adjust  
[1:07:16] Dispensed 0.001035 mL of Base (0.5 M KOH)  
[1:07:22] Stepping pH = 10.23  
[1:07:37] Stirrer speed set to 0  
[1:07:47] Datapoint id 76 collected  
[1:07:47] Charge balance equation is out by 50.0%  
[1:07:47] Stirrer speed set to 60  
[1:07:52] pH 10.22 -> 10.42  
[1:07:52] Using cautious pH adjust  
[1:07:52] Dispensed 0.001011 mL of Base (0.5 M KOH)  
[1:07:57] Stepping pH = 10.39  
[1:07:57] Dispensed 0.000212 mL of Base (0.5 M KOH)  
[1:08:02] Stepping pH = 10.40  
[1:08:02] Dispensed 0.000165 mL of Base (0.5 M KOH)  
[1:08:07] Stepping pH = 10.42  
[1:08:23] Stirrer speed set to 0  
[1:08:33] Datapoint id 77 collected  
[1:08:33] Charge balance equation is out by 31.5%  
[1:08:33] Stirrer speed set to 60  
[1:08:38] pH 10.42 -> 10.62  
[1:08:38] Using cautious pH adjust  
[1:08:38] Dispensed 0.001011 mL of Base (0.5 M KOH)  
[1:08:43] Stepping pH = 10.55  
[1:08:43] Dispensed 0.000376 mL of Base (0.5 M KOH)  
[1:08:48] Stepping pH = 10.59  
[1:08:48] Dispensed 0.000188 mL of Base (0.5 M KOH)  
[1:08:53] Stepping pH = 10.61  
[1:09:08] Stirrer speed set to 0  
[1:09:18] Datapoint id 78 collected  
[1:09:18] Charge balance equation is out by 21.6%  
[1:09:18] Stirrer speed set to 60  
[1:09:23] pH 10.60 -> 10.80  
[1:09:23] Using cautious pH adjust  
[1:09:24] Dispensed 0.001105 mL of Base (0.5 M KOH)  
[1:09:29] Stepping pH = 10.71  
[1:09:29] Dispensed 0.000729 mL of Base (0.5 M KOH)  
[1:09:34] Stepping pH = 10.77  
[1:09:34] Dispensed 0.000282 mL of Base (0.5 M KOH)  
[1:09:39] Stepping pH = 10.79  
[1:09:54] Stirrer speed set to 0  
[1:10:04] Datapoint id 79 collected  
[1:10:04] Charge balance equation is out by 5.1%  
[1:10:04] Stirrer speed set to 60  
[1:10:09] pH 10.78 -> 10.98  
[1:10:09] Using charge balance adjust

Sample name: **M16\_octanol**  
Assay name: **pH-metric high logP**  
Assay ID: **18C-01007**  
Filename: **C:\Sirius\_T3\Mehtap\20180228\_exp28\_logP\_T3-2\18C-01007\_M16\_octanol\_pH-metric high logP.t3r**

Experiment start time: **3/1/2018 9:25:34 AM**  
Analyst: **Pion**  
Instrument ID: **T312060**

## Experiment Log (continued)

[1:10:09] Dispensed 0.002705 mL of Base (0.5 M KOH)  
[1:10:30] Stirrer speed set to 0  
[1:10:40] Datapoint id 80 collected  
[1:10:40] Charge balance equation is out by -11.6%  
[1:10:40] Stirrer speed set to 60  
[1:10:45] pH 10.96 -> 11.16  
[1:10:45] Using charge balance adjust  
[1:10:45] Dispensed 0.003622 mL of Base (0.5 M KOH)  
[1:11:05] Stirrer speed set to 0  
[1:11:15] Datapoint id 81 collected  
[1:11:15] Charge balance equation is out by -20.9%  
[1:11:15] Stirrer speed set to 60  
[1:11:20] pH 11.12 -> 11.32  
[1:11:20] Using cautious pH adjust  
[1:11:21] Dispensed 0.002469 mL of Base (0.5 M KOH)  
[1:11:26] Stepping pH = 11.21  
[1:11:26] Dispensed 0.002140 mL of Base (0.5 M KOH)  
[1:11:31] Stepping pH = 11.29  
[1:11:31] Dispensed 0.000729 mL of Base (0.5 M KOH)  
[1:11:36] Stepping pH = 11.31  
[1:11:51] Stirrer speed set to 0  
[1:12:01] Datapoint id 82 collected  
[1:12:01] Charge balance equation is out by -7.8%  
[1:12:01] Stirrer speed set to 60  
[1:12:06] pH 11.31 -> 11.51  
[1:12:06] Using charge balance adjust  
[1:12:07] Dispensed 0.007385 mL of Base (0.5 M KOH)  
[1:12:27] Stirrer speed set to 0  
[1:12:37] Datapoint id 83 collected  
[1:12:37] Charge balance equation is out by -18.4%  
[1:12:37] Stirrer speed set to 60  
[1:12:42] pH 11.48 -> 11.68  
[1:12:42] Using cautious pH adjust  
[1:12:42] Dispensed 0.005386 mL of Base (0.5 M KOH)  
[1:12:47] Stepping pH = 11.57  
[1:12:47] Dispensed 0.004586 mL of Base (0.5 M KOH)  
[1:12:53] Stepping pH = 11.65  
[1:12:53] Dispensed 0.001787 mL of Base (0.5 M KOH)  
[1:12:58] Stepping pH = 11.67  
[1:13:13] Stirrer speed set to 0  
[1:13:23] Datapoint id 84 collected  
[1:13:23] Charge balance equation is out by -8.5%  
[1:13:23] Stirrer speed set to 60  
[1:13:28] pH 11.67 -> 11.87  
[1:13:28] Using charge balance adjust  
[1:13:29] Dispensed 0.017074 mL of Base (0.5 M KOH)  
[1:13:49] Stirrer speed set to 0  
[1:13:59] Datapoint id 85 collected  
[1:13:59] Charge balance equation is out by -11.5%  
[1:13:59] Stirrer speed set to 60  
[1:14:04] pH 11.85 -> 12.05  
[1:14:04] Using charge balance adjust  
[1:14:05] Dispensed 0.025823 mL of Base (0.5 M KOH)  
[1:14:25] Stirrer speed set to 0  
[1:14:35] Datapoint id 86 collected  
[1:14:35] Charge balance equation is out by -9.9%  
[1:14:35] Argon flow rate set to 0  
[1:14:39] Titrator arm moved over Titration position  
[1:15:00] The autoloader failed to pick at location "Sample position"